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Barry Arthur Page

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POSITRONIUM SCATTERING BY HYDROGEN AND HELIUM ATOMS

by

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ABSTRACT

There have been considerable differences between existing theoretical and experimental results for the very low energy scattering and annihilation of an ortho-positronium atom by a helium atom. Thus, there is a need to obtain more accurate theoretical results for the ortho-positronium-helium system. In this work the Kohn variational principle was used in an attempt to determine the scattering length. In the past, variational principles have played a significant role in atomic scattering theory. It is demonstrated in this thesis that the Kohn variational principle gives results that are difficult to relate to the scattering properties of this system. The use of this principle involved selecting a suitable trial wavefunction containing linear and non-linear parameters.

The trial wavefunction was inserted in an integral expression for the scattering length and the parameters determined by applying the variational technique. Difficulties were encountered that manifested themselves as irregular behaviour of the scattering length values. This irregular behaviour appears to be primarily due to the use of an inexact helium ground state wavefunction in the calculations. Modifications of various procedures suggested by Peterkop and Rabik (1971) and by Houston and Drachman (1971a, 1971b) were applied to this system.

The trial wavefunction obtained from this method was then used to calculate the effective charge (related to the annihilation rate) of the ortho-positronium-helium system. All the numerical calculations were carried out using the DEC-PDP10 and the CDC-CYBER 73 (originally of the CDC6400 series) at the University of Western Ontario.

Due to the erratic behaviour of the Kohn scattering length values a rigorous interpretation of the numerical results could not be made. Interpretations of the numerical results based on non-rigorous criteria gave values of the scattering length ranging from $2.33a_o$ to $1.0a_o$ with corresponding singlet effective charges of 0.011 and 0.12 respectively. It is felt that more accurate helium ground state wavefunctions must be used in order to obtain better estimates of the scattering length.

A similar calculation was performed on the zero-energy scattering of a positronium atom by a hydrogen atom. Here the scattering length was estimated to be $2.474a_o$ for the Antisymmetric case. Irregular behaviour of the scattering length values prevented reliable estimates to be carried out for the Symmetric case. This irregular behaviour is presumably due to the fact that the normal Kohn method does not provide a bound of the scattering length values obtained since in this case the projectile and target form a composite bound state.

Modifications to allow for this situation were considered to be beyond the scope of this thesis.

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CHAPTER 1

GENERAL REVIEW

1.1 Introduction

Positronium (Ps) is the bound state of a positron (e^+) and an electron (e^-). It may be regarded as being the lightest of the hydrogen-like atoms. There are many review articles on the properties of Ps (for example, Fraser (1968a) and the references contained therein). Some of the salient features of Ps are outlined below.

Ortho-positronium (o-Ps), the triplet state of Ps, corresponds to the case when the spins of the e^+ and e^- are parallel. It has a natural annihilation rate (annihilating into three photons) of $\lambda_o=0.71\times10^7$ sec^{-1}. Para-positronium (p-Ps), the singlet state of Ps, corresponds to the situation where the spins of the e^+ - e^- pair are anti-parallel. P-Ps has $\lambda_o=0.8\times10^{10}$ sec^{-1} (annihilating into two photons).

It is generally considered that the o-Ps lifetime may be shortened by various processes which convert it into p-Ps. These are known as quenching processes (Ore (1949), Fraser (1968a)). In particular, the mode of quenching of o-Ps in helium (He) gas is believed to consist mainly of the pick-off process. Here the e^+ of o-Ps may, during a collision, annihilate with an atomic e^- with which

it forms a singlet spin state. However, at high densities of He gas and low density He liquid, the observed annihilation rate of o-Ps is $\simeq 1.1 \times 10^7$ sec^{-1} which is quite close to the vacuum annihilation rate (Fraser (1968a)). A model has been presented suggesting that this is due to bubbles being formed around the o-Ps in He and there is considerable experimental evidence to support this view (Ferrel (1957), Briscoe, Choi and Stewart (1968), Hernandez and Choi (1969), Canter (1970)).

Another mode of quenching is known as conversion quenching. It is possible only in collisions of o-Ps with an atom or molecule which has one or more unpaired e^- (for example, hydrogen (H), nitric oxide (NO), oxygen (O_2)). Here by exchanging the unpaired e^- of the target atom with the e^- in the Ps atom, o-Ps may be converted to p-Ps. That is, this process is a pure exchange or rearrangement interaction (Ferrel (1958), Wallace (1960), Fraser (1961)).

1.2 Review Of Experimental Results

Important parameters needed to describe the very low energy effects in He are $^1Z_{eff}$ (the singlet effective charge) and a (the scattering length). Values of $^1Z_{eff}$ calculated from various experimental results range from 0.118 ± 0.011 (Duff and Heymann (1962)) to 0.25 ± 0.06 (Roellig and Kelly (1967)) in the o-Ps-He system. Fraser (1968a) deduced $^1Z_{eff} = 0.180 \pm 0.016$ from the data of Beers

and Hughes (1968). Roellig and Kelly (1967) used a value of $a = 2.1a_o$ (a_o = Bohr radius = 0.53×10^{-8}cm) and found reasonable consistency with their experimental results on cavities in o-Ps-He scattering. Canter (1970) found that the value of $a = (1.46 \pm 0.08)a_o$ described his experimental results for o-Ps scattering very well. From the results of Canter it was found that $^1Z_{eff} = 0.13 \pm 0.01$.

In the Ps-H system an analogy can be made with Ps scattering by NO, since NO has a single unpaired e^-. Earlier experimental results for the quenching cross section gave a value of $0.16\pi a_o^2$, assuming thermalized o-Ps (Heymann, et al (1961)). Fraser (1968a) pointed out that this result indicated that the quenching process is by conversion since the cross section is of the order of atomic areas. More recently, Tao, et al (1972) measured the quenching rate of o-Ps in NO. Using their value obtained together with the value for the velocity of thermalized o-Ps (8.2×10^6cm/sec) the cross section was calculated to be $7.7 \times 10^{-3}\pi a_o^2$.

1.3 Review Of Theoretical Results

On the theoretical side, Massey and Mohr (1954) surveyed the interaction of Ps with various gases using the Born approximation. For the Ps-H system they obtained $\sigma_t = 230\pi a_o^2$ (total cross section) at zero energy. Fraser (1961), using a static approximation, calculated phase

shifts and elastic cross sections for the scattering of low-energy Ps by H atoms. He obtained $a_+ = 13.4a_o$ for the symmetric case and $a_- = 1.84a_o$ for the anti-symmetric case. Here $\sigma_t = 192\pi a_o^2$, $\sigma_p = 33.8\pi a_o^2$ (conversion cross section) and $\sigma_p/\sigma_t = 0.176$. A similar calculation by Fraser and Kraidy (Fraser (1962), Fraser and Kraidy (1966), Fraser (1968b), Kraidy (1969, private communication)) was performed on the o-Ps-He system.

However, the ground state wavefunction of He is not known in a concise analytical form. As a result of this, additional terms appeared in the variational calculations when approximate ground state target wavefunctions are used. Fraser and Kraidy used the single parameter Hylleraas wavefunction and considered two different methods of treating this wavefunction in the calculations. One method consisted of retaining all of the additional terms in the calculations and gave values of $a = 1.88a_o$ with $^1Z_{eff} = 0.033$. In the other approach, all of the additional terms are neglected resulting in values of $a = 1.72a_o$ with $^1Z_{eff} = 0.042$. These two approaches will be considered in greater detail in Chapter 3.

Fraser (1962) also considered the simplest case where the scattering wavefunction was a plane wave (that is, no distortion or interaction effects between the Ps and He). Here the unsymmetrized version of the wavefunction of course gives $^1Z_{eff} = 0.5$ and the anti-

symmetrized wavefunction gave $^1Z_{eff} = 0.36$.

In earlier papers, Ferrel (1956, 1957) pointed out that there are basically two counter-acting forces acting between the Ps and the He atom, namely, the attractive Van der Waals force and the repulsive force arising from the fact that the two e^-s of the He atom form a closed shell. He further pointed out that this repulsive force should be the main reason for the formation of the long-lived component in liquid He, whereas the Van der Waals force works against this effect.

The low results of Fraser and Kraidy for $^1Z_{eff}$ compared with the experimental values stimulated Barker and Bransden (1968, 1969) to consider an approximation that allowed for the long-range Van der Waals force acting between the neutral atoms into the static-exchange approximation for the o-Ps-He system. They obtained $a = 1.61a_o$ and $^1Z_{eff} = 0.048$. Since these results for $^1Z_{eff}$ were still in poor agreement with experimental ones, it was felt that short-range effects were important (Bransden (1969)). Drachman and Houston (1970) devised a simplified model for o-Ps-He scattering which contained short-range correlation terms. Values of $a = 1.39a_o$ and $^1Z_{eff} = 0.10$ were obtained from their simplified model using a differential equation technique and also by the Kohn variational method. Their results demonstrated the importance of the short-range correlations.

1.4 Scope Of Thesis

All this work has stimulated the undertaking of an elaborate zero-energy variational calculation . Chapter 2 outlines the general procedures used in this work. However, certain aspects of this formalism break down when approximate ground state target wavefunctions are used. Chapter 3 gives specific details of the o-Ps-He system in which two different target ground state wavefunctions are considered. Certain modifications of the standard Kohn procedure are described here. Various considerations of Ps scattering by a H atom are also given in Chapter 3.

All the results obtained from these calculations are given in Chapter 4. Finally, various conclusions that resulted from this work are presented in Chapter 5. Several Appendices are included which contain details of the numerical calculations involved, and discussions of integrals too long for the main text.

CHAPTER 2

FORMULATION

2.1 Introduction

The Schrodinger equation for the system of Ps and a target atom is

$$(H-E)\ \Psi = 0 \qquad \text{.....(2.1)}$$

where H is the Hamiltonian of the system with wavefunction, Ψ, and corresponding energy E. It is assumed that the target nucleus is "infinitely massive" compared with the e^+ and e^-s and is treated as being fixed at the origin. Atomic units will be used in which $\hbar=1$, $m_e=1/2$, $e^2=2$, the energy is thus in rydbergs (1 rydberg= 13.6eV), and the unit of length is a_o (the Bohr radius = 0.53×10^{-8} cm). Here $2\pi\hbar$ is Planck's constant, m_e is the mass of an e^- , and e is the electronic charge.

For the case of a He atom as the target atom, the Hamiltonian describing the system is

$$H = -(\hbar^2/2m_e)(\nabla_1^2+\nabla_2^2+\nabla_3^2+\nabla_p^2) \quad -2e^2/r_1-2e^2/r_2-2e^2/r_3$$
$$+2e^2/r_p+e^2/|\vec{r}_1-\vec{r}_2|+e^2/|\vec{r}_1-\vec{r}_3|+e^2/|\vec{r}_2-\vec{r}_3|-e^2/|\vec{r}_1-\vec{r}_p|$$
$$-e^2/|\vec{r}_2-\vec{r}_p|-e^2/|\vec{r}_3-\vec{r}_p|$$

which, using atomic units, becomes

$$H = -\nabla_1^2 - \nabla_2^2 - \nabla_3^2 - \nabla_p^2 - 4/r_1 - 4/r_2 - 4/r_3 + 4/r_p + 2/|\vec{r}_1 - \vec{r}_2|$$
$$+2/|\vec{r}_1 - \vec{r}_3| + 2/|\vec{r}_2 - \vec{r}_3| - 2/|\vec{r}_1 - \vec{r}_p| - 2/|\vec{r}_2 - \vec{r}_p|$$
$$-2/|\vec{r}_3 - \vec{r}_p| \qquad \text{.....(2.2)}$$

Here the subscripts 1,2,3 refer to the e^- coordinates and p refers to the e^+ coordinate. The sign $\rightarrow$ denotes a vector quantity and r or $|\vec{r}|$ denotes the scalar magnitude of $\vec{r}$. Also, the energy of the system may be written (in atomic units) as

$$E = (1/2)k^2 - 1/2 + E_{He} \qquad \text{.....(2.3)}$$

where $(1/2)k^2$ is the kinetic energy of the Ps with k being the wave number, E_{He} represents the ground state energy of the He atom, and the ground state energy of the Ps is -1/2.

With the position of the e^- in the Ps atom represented by the coordinate r_1, the normalized Ps ground state wavefunction ϕ_1, satisfies

$$(-2\nabla_{\rho_1}^2 - 2/\rho_1)\phi_1 = -\phi_1/2$$

with

$$\phi_1 = e^{-\rho_1/2}/(8\pi)^{\frac{1}{2}}, \quad \vec{\rho}_1 = \vec{r}_1 - \vec{r}_p \qquad \text{.....(2.4)}$$

If the positions of the e^-s in the He atom are represented by r_2 and r_3 respectively then the He ground state wavefunction, ψ_{23}, satisfies

$$(-\nabla_2^2-\nabla_3^2-4/r_2-4/r_3+2/|\vec{r}_2-\vec{r}_3|)\psi_{23} = E_{He}\psi_{23}$$

.....(2.5)

When the target atom is a H atom, the Hamiltonian describing the system is

$$H=-(\hbar^2/2m_e)(\nabla_1^2+\nabla_2^2+\nabla_p^2) -e^2/r_1-e^2/r_2 +e^2/r_p$$

$$+e^2/|\vec{r}_1-\vec{r}_2| -e^2/|\vec{r}_1-\vec{r}_p| -e^2/|\vec{r}_2-\vec{r}_p|$$

which (using atomic units) becomes

$$H = -\nabla_1^2-\nabla_2^2-\nabla_p^2 -2/r_1-2/r_2+2/r_p+2/|\vec{r}_1-\vec{r}_2| -2/|\vec{r}_1-\vec{r}_p|$$

$$-2/|\vec{r}_2-\vec{r}_p| \qquad .....(2.6)$$

Since the ground state energy of H is -1, the energy of the system (in atomic units) is

$$E = k^2/2-3/2 \qquad .....(2.7)$$

Here the normalized H ground state wavefunction, ψ_2, satisfies

$$(-\nabla_2^2-2/r_2)\psi_2 = -\psi_2$$

where

$$\psi_2 = e^{-r_2}/(\pi)^{\frac{1}{2}} \qquad .....(2.8)$$

Only zero-kinetic energy (k=0) of the Ps atom will be considered. Solutions of equation (2.1) are sought such that the wavefunction, Ψ, has the asymptotic form

$$\Psi \rightarrow \phi_1 \psi(-1+a/\sigma_1) \quad \text{as } \sigma_1 \rightarrow \infty \qquad \text{.....(2.9)}$$

where $\vec{\sigma}_1=(\vec{r}_1+\vec{r}_p)/2$ is the center of mass coordinate of the Ps atom; ϕ_1, and ψ are the ground state wavefunctions of the Ps atom and the target atom respectively, and a is the scattering length.

2.2 Variational Method

In a variational calculation, Ψ is replaced by a trial wavefunction, Ψ_t. Ψ_t contains various linear and non-linear parameters which are adjusted to give a stationary value for an integral expression. In this work the Kohn variational method is used. Provided no composite projectile-target bound state exists, the Kohn variational principle gives an upper bound on the true scattering length, a, at zero kinetic energy of the projectile (Spruch and Rosenberg(1960)). The Kohn method is used rather than the Hulthén method because better results are obtained from the Kohn method (Spruch and Rosenberg (1959); Rosenberg, Spruch and O'Malley (1960)).

Here

$$a \leq a_K = a_t + (1/4\pi)(2m_p/\hbar^2)\, I_t \qquad \text{.....(2.10)}$$

where a_K is the Kohn scattering length, a_t is the trial scattering length, m_p is the mass of Ps. I_t is given by

$$I_t = \int \Psi_t\, (H-E)\, \Psi_t\, d\tau \qquad \text{.....(2.11)}$$

where H is the Hamiltonian of the system with corresponding energy E, and $d\tau$ represents integration over the coordinates of the e^+ and all the e^-s. Equation (2.10), using atomic units, reduces to

$$a \leq a_K = a_t + I_t/2\pi \qquad \text{.....(2 .12)}$$

The inequality (2.12) is not rigorously correct when an approximate ground state target wavefunction is used. This inequality was established by showing that the neglected term involving the square of the difference between the trial scattering wavefunction used and the true scattering wavefunction in the expression for a gave a negative contribution in the case when an exact ground state target wavefunction is used (Spruch and Rosenberg (1960)). However, the contribution of these neglected terms although always finite cannot be ascertained when an approximate ground state target wavefunction is used. As better and better approximations to the ground state target wavefunction are used it is felt that these contributions would become less important. This conclusion is illustrated by the work of Peterkop and Rabik (1971). Unfortunately, for the o-Ps-He system the use of extremely good approximations to the ground state He wavefunctions involves rather lengthy and very expensive calculations. In the present work, only two rather simple approximations to ψ_{23} (equation (2.5)) which are given in Chapter 3 were used in the Kohn method.

Basically, the Kohn procedure is as follows. Suppose that the trial wavefunction Ψ has n linear parameters, b_i, i=1,2 ... n, with $b_1 = a_t$. According to the Kohn principle the quantity, a_K, given by equation (2.12) may be made stationary with respect to variations of all the parameters including a_t. That is

$$\partial I_t/\partial a_t = -2\pi, \quad \partial I_t/\partial b_i = 0, \; i=2,3...n \qquad .....(2.13)$$

If the variation is restricted to the linear parameters, then from these equations, a set of n simultaneous linear equations is produced. These equations may be solved by the usual standard methods involving either inversion of the appropriate coefficient matrix or by Gaussian elimination.

Ψ_t also contains some non-linear parameters. Here a "trial and error" method may be adopted where the values of the non-linear parameters are adjusted to give the best results (Rosenberg, Spruch and O'Malley (1960), Spruch (1961)). The particular choice of Ψ_t used will be given in the next chapter.

2.3 Effective Charge

Only the o-Ps-He system is considered. For this system the singlet effective charge, $^1Z_{eff}$, may be regarded as being a measure of the probability that the e^+ is at the location of one of the He e^-s with which it

forms a singlet spin state (Fraser (1968a)). It is directly related to the annihilation rate (quenching rate) of o-Ps in He (Fraser (1968a)). Quantum electrodynamical formulations of similar systems have been studied (Ferrel (1956), Chang Lee (1958), Wallace (1960), Neamtan et al (1962)).

Following Fraser and Kraidy (1966) the wavefunction is projected on the spin singlet function of the e^+ and e^- (at position r_1) to get

$$\Phi(\vec{r}_p;\vec{r}_1;\vec{r}_2,s_2;\vec{r}_3,s_3) = (\chi_o^o(s_p,s_1),\Psi) \quad .....(2.14)$$

where s_p is spin coordinate of e^+ and s_1,s_2,s_3 those of the e^-s respectively. It may be shown that

$${}^1Z_{eff} = 3 \sum_{\substack{s_2 \\ s_3}} \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 \, |\Phi(\vec{r}_p;\vec{r}_1;\vec{r}_2,s_2;\vec{r}_3,s_3)|^2_{\vec{r}_p=\vec{r}_1} \quad .....(2.15)$$

At present, there are no known variational principles for calculating ${}^1Z_{eff}$. However, it is assumed that wavefunctions obtained from variational principles for scattering lengths are adequate for ${}^1Z_{eff}$ calculations.

2.4 Summary

To obtain a description of the zero-energy scattering of Ps by an atom, the Kohn variational method outlined above is employed. This method has the property that the difference between the exact scattering length and the variationally determined scattering length is proportional

to the square of the relative error between the trial wavefunction used and the exact wavefunction (Spruch (1961)). However, inherent difficulties arise when an inexact ground state target wavefunction is used. In such cases rigorous statements about the variationally determined scattering length cannot be made when the Kohn principle is used. Further consideration of this problem are given in Chapter 3.

Since annihilation of a e^+ and e^- takes place when the distance between them is within a Compton wavelength ($0.38 \times 10^{-12} m = a_o/137$) this can be considered as a point interaction for atomic processes (Wallace (1960), Bransden (1969)). Thus the wavefunction calculated variationally may be used to calculate the annihilation parameters. However, the annihilation parameters calculated (namely, $^1Z_{eff}$ in this case) may be considered to have approximately the same degree of accuracy as that of the scattering wavefunctions.

CHAPTER 3

METHOD OF SOLUTION

3.1 Introduction

Only the elastic channel is open at zero energy. In this case (ignoring annihilation) the trial wavefunction, Ψ_t, chosen must satisfy the asymptotic form given by equation (2.9) of the true wavefunction, Ψ. In this work, the trial wavefunction is chosen to be a simple product of the ground state wavefunctions of target and projectile together with a function termed the scattering wavefunction.

In particular the trial wavefunction for the o-Ps-He system is taken to be of the form

$$\Psi_t = (1/(3)^{\frac{1}{2}})(\phi_1\psi_{23}F_1\chi_1^1(p,1)\chi_o^o(2,3) + \phi_2\psi_{13}F_2\chi_1^1(p,2)\chi_o^o(3,1) + \phi_3\psi_{12}F_3\chi_1^1(p,3)\chi_o^o(1,2)) \qquad \text{.....(3.1)}$$

where the ϕ's and ψ's are the appropriate ground state wavefunctions of Ps and He defined in equations (2.4) and (2.5) respectively. Here the F's represent the scattering wavefunction having the asymptotic form

$$F_1 \rightarrow -1 + a_t/\sigma_1 \quad \text{as } \sigma_1 \rightarrow \infty \qquad \text{.....(3.2)}$$

where $\vec{\sigma}_1 = (\vec{r}_1+\vec{r}_p)/2$. F_2 corresponds to F_1 where the coordinates $\vec{r}_1$ and $\vec{r}_2$ are interchanged. F_3 corresponds to F_1 where the coordinates $\vec{r}_1$ and $\vec{r}_3$ are interchanged. $\chi_1^1(p,1),\chi_1^1(p,2)$ and $\chi_1^1(p,3)$ represent the Ps triplet spin function. $\chi_o^o(2,3),\chi_o^o(1,3)$ and $\chi_o^o(1,2)$ represent the He singlet spin function. This trial wavefunction, Ψ_t, satisfies the Pauli Exclusion Principle, which requires the wavefunction to be antisymmetric with respect to the interchange of the e^- .

Using the orthogonality properties of the Pauli spin functions it may be shown that the integral

$$I_t = \int \Psi_t \, (H - E) \, \Psi_t d\tau$$

using Ψ_t given by equation (3.1) becomes

$$I_t = \int \phi_1 \Psi_{23} F_1 \, (H-E)(\phi_1 \Psi_{23} F_1 - \phi_2 \Psi_{13} F_2) d\tau \qquad \text{.....(3.3)}$$

Proceeding in a similar fashion for the Ps-H system as for the o-Ps-He system above, trial wavefunctions of the form

$$\Psi_{\pm} = (1/(2)^{\frac{1}{2}}) \, (\phi_1 \Psi_2 F_1 \pm \phi_2 \Psi_1 F_2) \qquad \text{.....(3.4)}$$

are constructed. Here the + and - signs refer to the space symmetric and antisymmetric cases respectively. The ϕ's and Ψ's are the appropriate ground state wavefunctions of Ps and H defined in equations (2.4) and (2.8) respectively.

With this form for the trial wavefunction the integral

$$I_t = \int \Psi_t (H-E) \Psi_t d\tau$$

reduces to

$$I_t = \int \phi_1 \psi_2 F_1 (H-E)(\phi_1 \psi_2 F_1 \pm \phi_2 \psi_1 F_2) d\tau \qquad .....(3.5)$$

3.2 Trial Wavefunction

For both the o-Ps-He and the o-Ps-H systems the choice of the scattering wavefunction, F_1, is

$$F_1 = v_1/\sigma_1 + a_t\, w_1/\sigma_1 + \sum_\ell b_\ell f_\ell^{(1)}/\sigma_1 + \sum_j c_j \chi_j^{(1)} \qquad .....(3.6)$$

where $\vec{\sigma}_1 = (\vec{r}_1 + \vec{r}_p)/2$ is the centre of mass coordinate of the Ps. Here

$$v_1 = -\sigma_1 , \qquad w_1 = 1 - e^{-\delta\sigma_1} ,$$

$$f_\ell^{(1)} = \sigma_1^\ell e^{-\delta\sigma_1} , \quad \chi_j^{(1)} = e^{\beta\rho_1} e^{-\gamma r_1} e^{-\eta r_p}\, \rho_{1j}^{m_j}\, r_{1j}^{q_j}\, r_p^{h_j} \qquad .....(3.7)$$

with $\vec{\rho}_1 = \vec{r}_1 - \vec{r}_p$; $\vec{r}_1$ and $\vec{r}_p$ being the e^- and e^+ coordinates of the Ps atom. Note that b_ℓ and c_j are linear parameters of $f_\ell^{(1)}$ and $\chi_j^{(1)}$ respectively and the $\sum_\ell$ and $\sum_j$ symbols denote a sum of such terms. Furthermore, $f_\ell^{(1)}$ contains a non-linear parameter, δ, and $\chi_j^{(1)}$ contains the non-linear parameters, β, γ, and η.

In this expression for F_1, v_1 represents the plane wave term. All the other terms have exponential factors so that they vanish at infinity. v_1 and w_1 contains the asymptotic form of F_1 for large projectile-target separations. The terms v_1, w_1 and $f_\ell^{(1)}$ make up the so-called static part of F_1 since they contain the projectile-target coordinate only. The term $\chi_j^{(1)}$ allows for short range correlation effects.

It is convenient to adopt the following notation:

$$(x,y) = \int \phi_1 \psi_{23}\, x^{(1)}(H-E)\phi_1 \psi_{23}\, y^{(1)} d\tau$$

$$- \int \phi_1 \psi_{23} x^{(1)}(H-E)\phi_2 \psi_{13} y^{(2)} d\tau \quad .....(3.8)$$

for the o-Ps-He equations; and

$$(x,y) = \int \phi_1 \psi_2 x^{(1)}(H-E)\phi_1 \psi_2 y^{(1)}\, d\tau$$

$$\pm \int \phi_1 \psi_2 x^{(1)}(H-E)\phi_2 \psi_1 y^{(2)} d\tau \quad .....(3.9)$$

for the Ps-H equations.

Substituting the form of F given by equation (3.6) into equation (3.3) results in

$$I_t = A + a_t B + a_t^2 C + \underline{D}\,\underline{b} + a_t \underline{E}\,\underline{b} + \underline{b}^T \underline{F}\,\underline{b}$$

$$+ \underline{R}\,\underline{c} + a_t \underline{H}\,\underline{c} + \underline{b}^T \underline{S}\,\underline{c} + \underline{c}^T \underline{K}\,\underline{c}$$

$$.....(3.10)$$

where $\underline{b}$ and $\underline{c}$ are column matrices with $\underline{b}^T$ and $\underline{c}^T$ their corresponding transposes. $\underline{D}$, $\underline{E}$ and $\underline{R}$ are row matrices.

$\underline{S}$ is a matrix with the same number of rows as $\underline{R}$ and the same number of columns as $\underline{b}$. $\underline{F}$ and $\underline{K}$ are square matrices.

Here

$$A = (v/\sigma, v/\sigma) \qquad \text{.....(3.11)}$$

$$B = (v/\sigma, w/\sigma) + (w/\sigma, v/\sigma) \qquad \text{.....(3.12)}$$

$$C = (w/\sigma, w/\sigma) \qquad \text{.....(3.13)}$$

The elements of the matrices indicated in equation (3.10) are

$$D_i = (v/\sigma, f_i/\sigma) + (f_i/\sigma, v/\sigma) \qquad \text{.....(3.14)}$$

$$E_i = (w/\sigma, f_i/\sigma) + (f_i/\sigma, w/\sigma) \qquad \text{.....(3.15)}$$

$$F_{ij} = (f_i/\sigma, f_j/\sigma) = F_{ji} \qquad \text{.....(3.16)}$$

$$R_i = (v/\sigma, \chi_i) + (\chi_i, v/\sigma) \qquad \text{.....(3.17)}$$

$$H_i = (w/\sigma, \chi_i) + (\chi_i, w/\sigma) \qquad \text{.....(3.18)}$$

$$S_{ij} = (f_i/\sigma, \chi_j) + (\chi_j, f_i/\sigma) \qquad \text{.....(3.19)}$$

$$K_{ij} = (\chi_i, \chi_j) = K_{ji} \qquad \text{.....(3.20)}$$

Using equation (3.10) in equation (2.13) gives a set of simultaneous linear equations:

$$2Ca_t + B + \underline{E}\,\underline{b} + \underline{H}\,\underline{c} = -2\pi \qquad \text{.....(3.21)}$$

$$\underline{E}a_t + \underline{D} + (\underline{F} + \underline{F}^T)\,\underline{b} + \underline{S}\,\underline{c} = 0 \qquad \text{.....(3.22)}$$

$$\underline{H}a_t + \underline{R} + \underline{S}\,\underline{b} + (\underline{K} + K^T)\,\underline{c} = 0 \qquad \text{.....(3.23)}$$

where $\underline{F}^T$ is the transpose of $\underline{F}$ and $\underline{K}^T$ the transpose of $\underline{K}$. Now $\underline{F}^T = \underline{F}$ and $K^T = \underline{K}$. Therefore, equations (3.22) and (3.23) become

$$\begin{bmatrix} 2\underline{F} & \underline{S} \\ \underline{S} & 2\underline{K} \end{bmatrix} \begin{bmatrix} \underline{b} \\ \underline{c} \end{bmatrix} = - \begin{bmatrix} \underline{D} \\ \underline{R} \end{bmatrix} - a_t \begin{bmatrix} \underline{E} \\ \underline{H} \end{bmatrix} \qquad \text{.....(3.24)}$$

Equations (3.21) and (3.24) may be solved either by a matrix inversion method or by Gaussian elimination techniques.

Note that with the Hulthen method, equations (2.13) are used except that $\partial I_t/\partial a_t = -2\pi$ is replaced by $I_t = 0$. That is, equation (3.21) is replaced by

$$A + Ba_t + Ca_t^2 + \underline{D}\,\underline{b} + a_t\,\underline{E}\,\underline{b} + \underline{b}^T\,\underline{F}\,\underline{b} + \underline{R}\,\underline{c} + a_t\,\underline{H}\,\underline{c}$$

$$+\underline{b}^T\,\underline{S}\,\underline{c} + \underline{c}^T\,\underline{K}\,\underline{c} = 0 \qquad \text{.....(3.25)}$$

Here equation (3.24) is solved by matrix inversion expressing $\underline{b}$ and $\underline{c}$ in terms of a_t. Substituting into equation (3.25) yields a quadratic equation in a_t which can be solved in the usual way.

Keeping in mind the notation given in equations (3.8) and (3.9) it can be shown that equations (3.10) through to equation (3.25) apply to both the o-Ps-He and Ps-H systems. However, the following considerations apply only to the o-Ps-He system regarding ${}^1Z_{eff}$. Using the choice of Ψ_t

given by equation (3.1), equation (2.15) reduces to

$$^1Z_{eff} = (1/2)\int(\phi_2^2\psi_{13}^2 F_2^2 - \phi_2\phi_3\psi_{13}\psi_{23}F_2F_3)_{\vec{r}_1=\vec{r}_p} d\vec{r}_2 d\vec{r}_3 d\vec{r}_p \qquad .....(3.26)$$

For convenience, let

$$\{x,y\} = \int(\phi_2^2\psi_{13}^2 x^{(2)}y^{(2)} - \phi_2\phi_3\psi_{13}\psi_{23}x^{(2)}y^{(3)})_{\vec{r}_1=\vec{r}_p} x d\vec{r}_2 d\vec{r}_3 d\vec{r}_p \qquad .....(3.27)$$

Then $^1Z_{eff}$ becomes, using equation (3.6),

$$^1Z_{eff} = (1/2)(A' + a_tB' + a_t^2C' + \underline{D}'\underline{b} + a_t\underline{E}'\underline{b} + \underline{b}^T\underline{F}'\underline{b} + \underline{R}'\underline{c} + a_t\underline{H}'\underline{c} + \underline{b}^T\underline{S}'\underline{c} + \underline{c}^T\underline{K}'\underline{c}) \qquad .....(3.28)$$

Here

$$A' = \{v/\sigma, v/\sigma\} \qquad .....(3.29)$$

$$B' = 2\{v/\sigma, w/\sigma\} \qquad .....(3.30)$$

$$C' = \{w/\sigma, w/\sigma\} \qquad .....(3.31)$$

and the matrix elements are given by

$$D_i' = 2\{v/\sigma, f_i/\sigma\} \qquad .....(3.32)$$

$$E_i' = 2\{w/\sigma, f_i/\sigma\} \qquad .....(3.33)$$

$$F_{ij}' = \{f_i/\sigma, f_j/\sigma\} = F_{ji}' \qquad .....(3.34)$$

$$R'_i = 2\{v/\sigma, \chi_i\} \qquad .....(3.35)$$

$$H'_i = 2\{w/\sigma, \chi_i\} \qquad .....(3.36)$$

$$S'_{ij} = 2\{f_i/\sigma, \chi_j\} \qquad .....(3.37)$$

$$K'_{ij} = \{\chi_i, \chi_j\} = K'_{ji} \qquad .....(3.38)$$

By using the values for the various linear and non-linear parameters of Ψ_t obtained from the variational calculation, $^1Z_{eff}$ can be calculated using equations (3.28) through to equation (3.38).

3.3 He Wavefunction

Unfortunately, the atomic ground state wavefunction of He is not known exactly. With e^- at $\vec{r}_2$ and $\vec{r}_3$ in the He atom, the He wavefunction, Ψ_{23}, is chosen to be of the form

$$\Psi_{23} = N_1 \sum_{i=1}^{M} u_i e^{-x_i r_2} e^{-y_i r_3} \qquad .....(3.39)$$

where N_1, u_i, x_i, y_i and M are constants. Now the He Hamiltonian is

$$H_{He_{23}} = -\nabla_2^2 - \nabla_3^2 - 4/r_2 - 4/r_3 + 2/|\vec{r}_2 - \vec{r}_3|$$

Hence,

$$(H_{He_{23}} - E_{He})\psi_{23} = N_1 \sum_{i=1}^{M} u_i e^{-x_i r_2} e^{-y_i r_3}((2x_i - 4)/r_2 + (2y_i - 4)/r_3 + 2/|r_2 - r_3| - x_i^2 - y_i^2 - E_{He}) \qquad .....(3.40)$$

Note that equation (3.39) deals only with a very restricted class of possible He wavefunctions. In particular, for this present work, only one class of functions is considered, namely, closed-shell wavefunctions without any correlation terms. Of this class, two functions were selected: the simple one parameter Hylleraas wavefunction (Hylleraas (1929)),

$$\Psi_{23} = (\mu^3/\pi)e^{-\mu(r_2+ r_3)} \qquad \text{.....(3.41)}$$

with μ=1.6875 and variational energy = $-2\mu^2$ rydbergs; and the three parameter Hartree-Fock type wavefunction (Green et al (1954))

$$\Psi_{23} = (N_2^2/4\pi)(e^{-\lambda r_2}+N_3 e^{-2\lambda r_2})(e^{-\lambda r_3}+ N_3 e^{-2\lambda r_3}) \qquad \text{.....(3.42)}$$

with N_2 =2.968466, λ =1.455799, N_3 =0.6 and variational energy = -5.72334 rydbergs.

3.4 Modifications Of The Kohn Method

The concern here is that, when an inexact ground state target wavefunction is used, the nature of the total contribution of the neglected terms relating a_K to a cannot be ascertained. Here it may be shown that (Houston (1973b))

$$a = a_t + (1/2\pi\Delta_1)(\int\Psi_t(H-E_{o_t})\Psi_t d\tau - \int\delta\Psi(H-E_o)\delta\Psi d\tau + (E_{o_t}-E_o)^2\int\Psi_t^2 d\tau) \qquad \text{.....(3.43)}$$

where

$$\Delta_1 = \int \psi_o \psi_{o_t} d\tau \ , \quad \delta\Psi = \Psi_t - \Psi \ .$$

ψ_o is the exact ground state target wavefunction with energy eigenvalue E_o; ψ_{o_t} being an approximation to ψ_o variationally obtained with variational energy E_{o_t}.

Performing the Kohn variation on the expression

$$a_K = a_t + I_t/2\pi$$

amounts to neglecting the terms involving $(\delta\Psi)^2$ and $(E_{o_t}-E_o)^2$ in equation (3.43). This also amounts to setting $\Delta_1 = 1$. It is easily demonstrated that the neglected terms do not give an infinite contribution contrary to the remark of Houston (1973b). Since the starting point of equation (3.43) dealt with finite quantities and all the quantities apart from the neglected terms are finite, it follows that the neglected terms collectively have a finite contribution.

Peterkop and Rabik (1971) demonstrated that the use of an approximate target ground state wavefunction may not lead to accurate results. Various variants of the standard Kohn procedure were used in which they included part of the neglected terms in the calculations. They observed that using the exact ground state energy of the target instead of the variational energy in some integrals of the calculation seemed to produce better results.

A "method of models" employed by Houston et al (1971a, 1971b) and Drachman (1972) incorporated to some extent the "successful variants" used by Peterkop and Rabik. This method amounts to replacing the complete Hamiltonian by a "model" Hamiltonian for which the approximate target ground state wavefunction is an exact solution. A modified version of the "method of models" has to be used for the o-Ps-He system since the projectile is not altogether distinguishable from the atomic e^- . This will be called the "Pseudo-Exact" (PE) case. Another alternative approach is to just use the inexact He wavefunction in the normal variational method with the complete Hamiltonian of the o-Ps-He system. This will be termed the "Inexact" (IE) case. In both cases E_{He} is replaced by the appropriate variational energy so that all the integrals will be finite.

For convenience, a parameter, Δ, is introduced into equation (3.40) such that $\Delta = 0$ for the PE case and $\Delta = 1$ for the IE case. That is, equation (3.40) becomes

$$(H_{He_{23}} - E_{He})\psi_{23} = \Delta N_1 \sum_{i=1}^{M} u_i e^{-x_i r_2} e^{-y_i r_3}((2x_i-4)/r_2 - x_i^2-y_i^2 + (2y_i-4)/r_3 + 2/|\vec{r}_2-\vec{r}_3| - E_{He}) \quad \ldots\ldots\ldots(3.44)$$

To illustrate how these two cases are applied to the o-Ps-He system, the matrix elements, F_{ij}, given by equation (3.16) will be used. Here

$$F_{ij} = \int \phi_1 \psi_{23} (f_i^{(1)}/\sigma_1)(H-E)\phi_1 \psi_{23} (f_j^{(1)}/\sigma_1) d\tau$$

$$- \int \phi_1 \psi_{23} (f_i^{(1)}/\sigma_1)(H-E)\phi_2 \psi_{13} (f_j^{(2)}/\sigma_2) d\tau$$

$$= F_{ij})_{\text{direct}} - F_{ij})_{\text{exchange}} \qquad \text{.....(3.45)}$$

The first term in the above expression has been called the "Direct term" and the second term has been labelled the "Exchange term". It is easy to show that the two cases will give the same values for $F_{ij})_{\text{direct}}$. That is,

$$F_{ij})^{PE}_{\text{direct}} = F_{ij})^{IE}_{\text{direct}} \qquad \text{.....(3.46)}$$

Furthermore, these matrix elements form a symmetric matrix.

Applying the PE case method to $F_{ij})_{\text{exchange}}$ operating through with the Hamiltonian on the right-hand side function $\phi_2 \psi_{13} f_j^{(2)}/\sigma_2$ gives matrix elements that will be denoted by $F_{ij})^R_{\text{exchange}}$. By performing the operation with the Hamiltonian on the left-hand side function $\phi_1 \psi_{23} f_j^{(1)}/\sigma_1)$ gives matrix elements that will be denoted by $F_{ij})^L_{\text{exchange}}$. However, neither the matrix elements, $F_{ij})^R_{\text{exchange}}$ nor $F_{ij})^L_{\text{exchange}}$ form a symmetric matrix.

Moreover,

$$F_{ij})^R_{\text{exchange}} \neq F_{ij})^L_{\text{exchange}} \qquad \text{.....(3.47)}$$

Now, by taking the average value of these two matrix elements, a symmetric matrix results. That is, for the

PE case, the matrix elements, $F_{ij})^{PE}_{exchange}$ will be defined by

$$F_{ij})^{PE}_{exchange} = (1/2)(F_{ij})^{R}_{exchange} + F_{ij})^{L}_{exchange}) \quad .....(3.48)$$

Equation (3.47) may be justified on the basis that when the complete Hamiltonian for the c-Ps-He system is used (as in the IE case), the matrix elements, F_{ij}, form a symmetric matrix. The matrix elements, $F_{ij})_{exchange}$, for the IE case will be denoted by $F_{ij})^{IE}_{exchange}$.

Peterkop and Rabik (1971) used a simple one parameter exponential function to represent the target ground state wavefunction for Hydrogen and calculated scattering lengths for various values of the exponential parameter. They considered four variants of the variational principle. A close study of their results revealed that over a wide range of values for the exponential parameter there was a "reasonable" convergence. The convergence was "reasonable" in the sense that the apparently converged value was not far from the value obtained using the exact target ground state wavefunction ignoring the irregular behaviour that frequently occured. In particular, this was observed in their variants 2 and 4 if the irregularities in the curves were ignored.

In the o-Ps-He system considered here, variant 1

corresponds to the IE case. Variant 2 corresponds to the IE case in which $D_k)^{IE}$, $E_k)^{IE}$, $R_k)^{IE}$ and $H_k)^{IE}$ are replaced by $D_k)^{PE}$, $E_k)^{PE}$, $R_k)^{PE}$ and $H_k)^{PE}$ respectively. Variant 3 corresponds to the PE case with the addition of the terms

$$(E_{o_t}-E_o)(\underline{D}''\underline{b} + a_t\underline{E}''\underline{b} + \underline{b}^T\underline{F}''\underline{b} + \underline{R}''\underline{c} + a_t\underline{H}''\underline{c} + \underline{b}^T\underline{S}''\underline{c} + \underline{c}^T\underline{K}''\underline{c}) \qquad .....(3.49)$$

Here

$$D_i'' = 2[v/\sigma, f_i/\sigma]$$

$$E_i'' = 2[w/\sigma, f_i/\sigma]$$

$$F_{i_j}'' = [f_i/\sigma, f_j/\sigma]$$

$$R_i'' = 2[v/\sigma, \chi_i]$$

$$H_i'' = 2[w/\sigma, \chi_i]$$

$$S_{i_j}'' = 2[f_i/\sigma, \chi_j]$$

$$K_{i_j}'' = 2[\chi_i, \chi_j]$$

with

$$[x,y] = \int \phi_1\psi_{23}x^{(1)}(\phi_1\psi_{23}y^{(1)} - \phi_2\psi_{13}y^{(2)})d\tau \qquad .....(3.50)$$

E_{o_t} is the appropiate variational energy of the approximate He ground state wavefunction used, E_o = -5.807448754 rydbergs (Frankowski and Pekeris (1966)).

Variant 4 is the same as variant 2 with the addition

of the terms given by equation (3.49).

These considerations will be used for all the expressions defined in equations (3.14) through to equation (3.20). Details of the numerical evaluation of all the expressions regarding the scattering length and also of the effective charge involve rather lengthy equations and are given in the Appendices.

3.5 Summary

In this formulation a trial wavefunction has been selected such that it has the correct asymptotic form. Correlation terms are introduced into the trial wavefunction to allow for any distortion of the Ps atom and other short-range effects. This is an extension of the calculations by Fraser (1961, 1962). It has been found that similar correlation terms play a very important role in the other zero-energy scattering processes (Houston and Moiseiwitsch (1968)).

The Kohn variational method that has been used here, although it always gives stationary scattering length values, will only give an upper bound to a for systems where no composite bound states of the projectile and target are possible. However, it has been established that the compound Positronium Hydride (PsH) forms a bound state (Lebeda and Schrader (1969), Houston and Drachman (1973)). This occurs only in the symmetric case of the Ps-H system. Modifications of the Kohn variational

method may be made to deal with this situation (Rosenberg, Spruch and O'Malley (1960)) but will not be considered here as these calculations for Ps-H are of an exploratory nature. It seems unlikely that any experiments will ever be performed on Ps-H scattering.

Difficulties arise in this work due to the use of an approximate He ground state wavefunction. Certain modifications of the Kohn method including the various methods of Peterkop and Rabik (1971) and of Houston and Drachman (1971a, 1971b) have been outlined to deal with this problem. It is possible that the correlation terms used in the trial wavefunction may reduce the errors that result from the use of an approximate target ground state wavefunction.

CHAPTER 4

RESULTS

4.1 Introduction

In all the calculations the scattering wavefunctions, F's, that are used have the form

$$F_1 = v_1/\sigma_1 + a_t w_1/\sigma_1 + \sum_\ell b_\ell f_\ell^{(1)}/\sigma_1 + \sum_j c_j \chi_j^{(1)} \qquad .....(4.1)$$

with

$$f_\ell^{(1)} = \sigma_1^\ell e^{-\delta\sigma_1} \qquad .....(4.2)$$

and

$$\chi_j^{(1)} = e^{\beta\rho_1}\, e^{-\gamma r_1}\, e^{-\eta r_p}\, \rho_1^{m_j}\, r_1^{q_j}\, r_p^{h_j} \qquad .....(4.3)$$

4.2 o-Ps-He System Using Hylleraas He Wavefunction

Calculations were first performed using the static approximation. This amounts to setting all the linear parameters c_j of the functions $\chi_j^{(1)}$, equal to zero. A few values of δ were tried and it was found that the scattering length value obtained was relatively insensitive to small changes of δ. Convergence was attained after three terms and the results using $\delta = 0.7$ are given in Table 1. These results agree quite well with those previously obtained by Fraser and Kraidy. There appears to be no sign of any irregular behaviour of the Kohn

TABLE 1

Static Results for o-Ps-He scattering using a one parameter Hylleraas ground state He wavefunction.

$\delta = 0.7$

(a) PE case

ℓ	a_K	a_t	Z
0	1.782	1.812	0.0443
1	1.777	1.926	0.0435
2	1.758	1.676	0.0414
3	1.754	1.775	0.0410

(b) IE case

ℓ	a_K	a_t	Z
0	1.911	1.915	0.0367
1	1.903	2.063	0.0355
2	1.883	1.807	0.0336
3	1.881	1.893	0.0333

scattering length values, a_K. That is, the Kohn method seems to give meaningful results in the static approximation.

Correlation terms of the type specified in equation (4.3) were then added such that

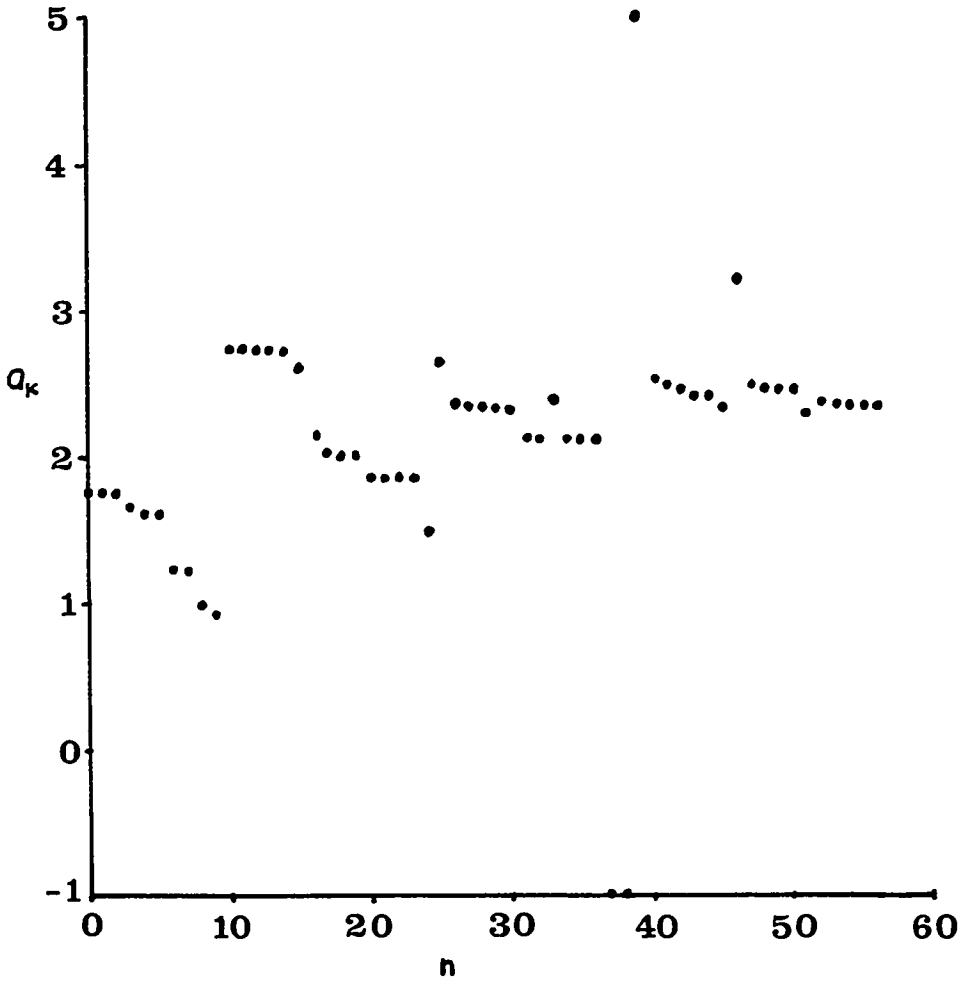
$$m_j + q_j + h_j \leq N \quad \text{with } N = 1,2,3... \quad .$$

After 10 correlation terms were added (that is, N = 2) the exponent parameters were varied. Over a wide range of values of γ and η there was very little change in a_K. However, a steady decrease in a_K was observed, as the correlation terms were added on, for small values of η (that is, η near 0) and for values of γ near 1. Furthermore, it was noticed that $\beta = 0.2$ gave lower values of a_K than both $\beta = 0.15$ and $\beta = 0.25$. Using the property that the value of a_K does not depend very much on the non-linear parameters when a large number of correlation terms are included (Schwartz (1961a), Drachman and Houston (1970)), suitable values were taken to be $\beta = 0.2$, $\gamma = 1.2$, $\eta = 0.1$ with $\delta = 0.7$.

More correlation terms were added to the wavefunction up to N = 5 (that is, 56 terms). Irregular behaviour of the scattering length, a_K, frequently occurred as shown in Figures 1 and 2. This type of behaviour has been reported to occur in similar variational calculations in other systems (Schwartz (1961a, 1961b), Peterkop and Rabik (1971), Houston (1973b)). This irregular behaviour of a_K

Figure 1

Results for the PE case of the o-Ps-He system using the one parameter Hylleraas He ground state wavefunction when the correlation terms were added on such that $h_j + q_j + m_j \leq N$.

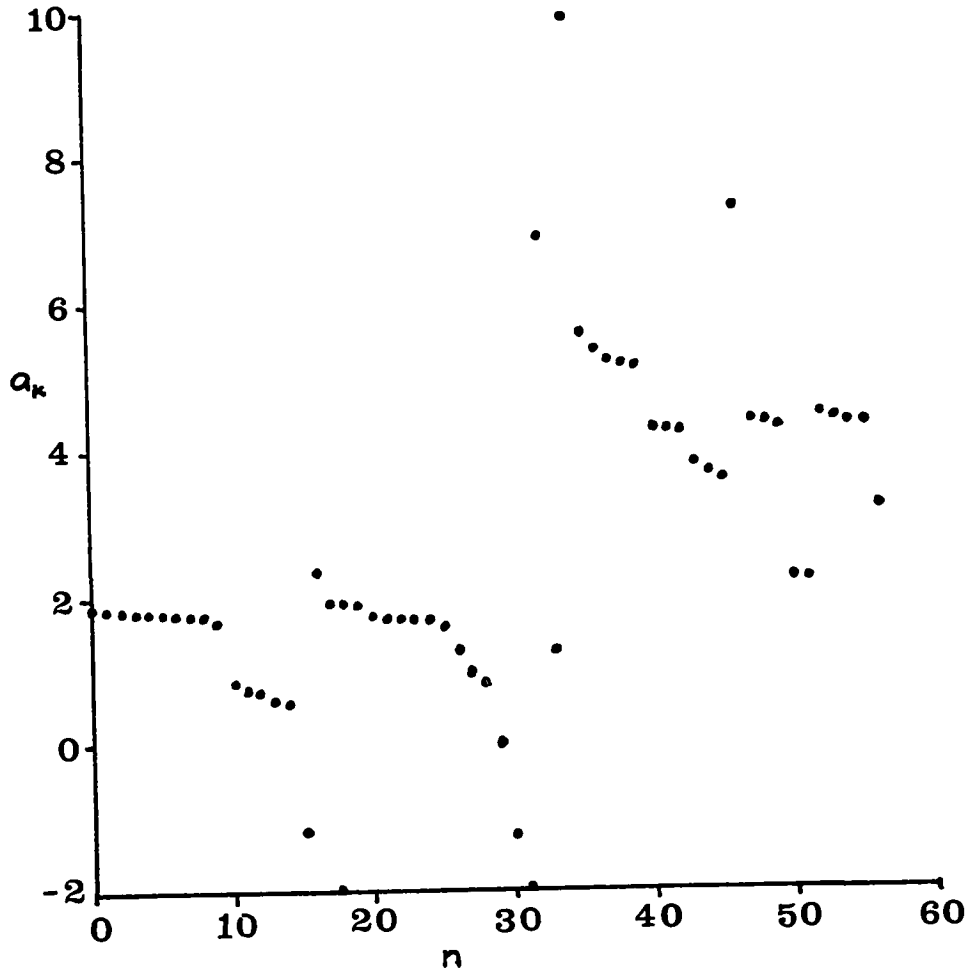


• refers to the Kohn scattering length, a_K.

n refers to the number of correlation terms used.

Figure 2

Results for the IE case of the o-Ps-He system using the one parameter Hylleraas He ground state wavefunction when the correlation terms were added on such that $h_j + q_j + m_j \leq N$.



• refers to the Kohn scattering length, a_K.

n refers to the number of correlation terms used.

has made an accurate determination of the exact scattering length value extremely difficult.

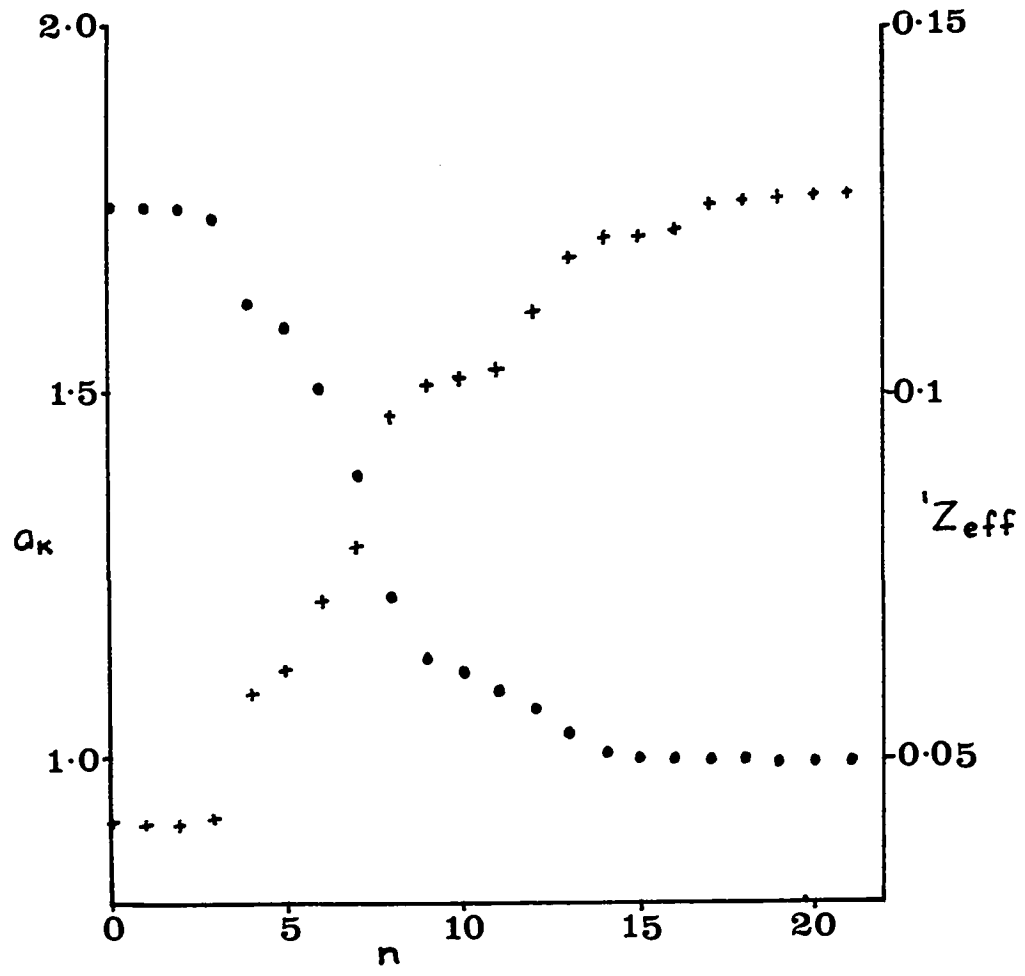
It was found that the value of a_K always decreased at first as the correlation terms were added on. From experimental findings, it is supposed that a_K should be greater than zero. With these considerations the following method was devised. Here, as the correlation terms were added on, if any term caused an irregular value of a_K to appear (that is, either much greater than the previous value of a_K or less than zero) it was not included at that point but re-cycled with the remaining correlation terms. Using this approach it was found that a_K seemed to converge as shown in Figures 3 and 4. Note that the addition of any one of the remaining first 56 correlation terms gave a value of a_K either much greater than 2.0 or less than zero. Tables 2 and 3 show how the linear coefficients of the scattering wavefunction, F, vary as the correlation terms are introduced.

For the PE case $a_K = 0.9902a_o$ with $a_t = 1.138a_o$ and $^1Z_{eff} = 0.127$; while for the IE case $a_K = 0.9824a_o$ with $a_t = 0.9672a_o$ and $^1Z_{eff} = 0.114$.

Another approach is to take the value of a_K on the flat portion of the curves of Figures 1 and 2. Here $a_K = 2.33a_o$, $a_t = 2.27a_o$ with $^1Z_{eff} = 0.011$ for the PE case; $a_K = 1.75a_o$, $a_t = 1.81a_o$ with $^1Z_{eff} = 0.037$ for the IE case.

Figure 3

Results for the PE case of the o-Ps-He system using the one parameter Hylleraas ground state wavefunction when selected correlation terms were added on such that irregular behaviour was avoided.



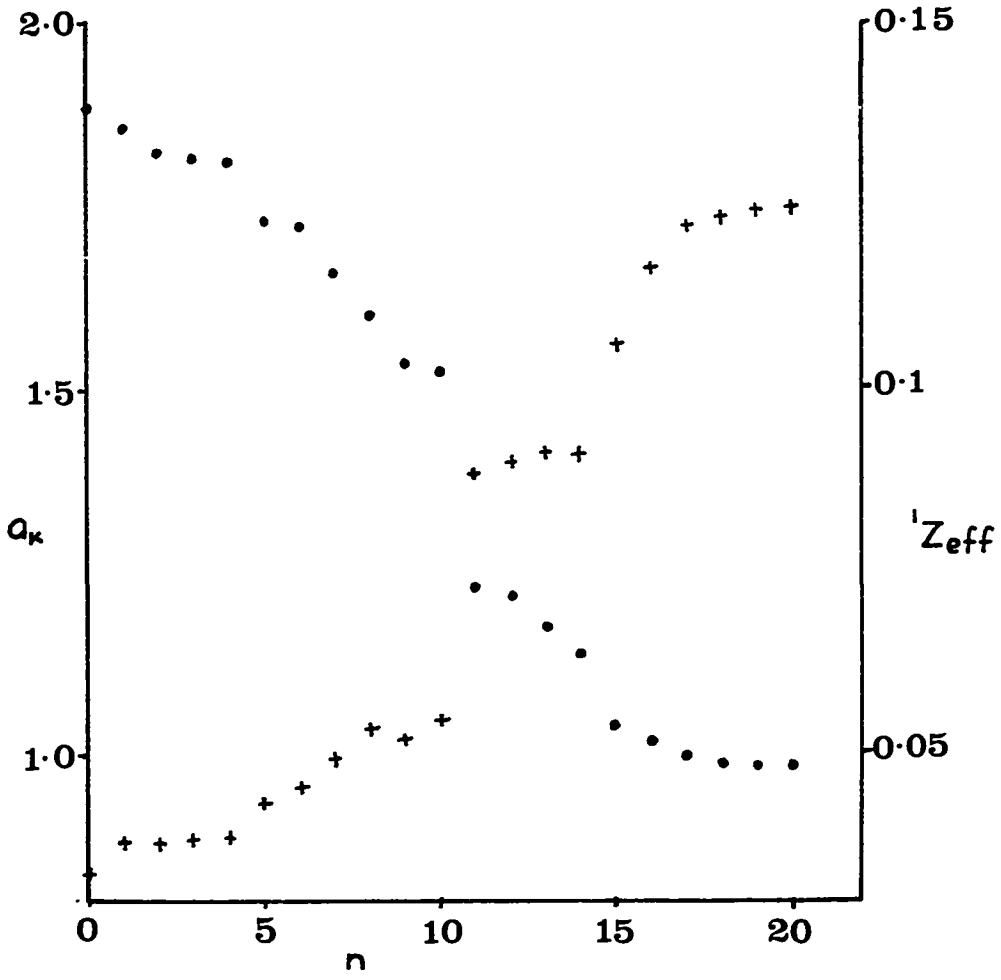
n refers to the number of correlation terms used.

• refers to the Kohn scattering length, a_K .

+ refers to the singlet effective charge, $^1Z_{eff}$.

Figure 4

Results for the IE case of the o-Ps-He system using the one parameter Hylleraas ground state wavefunction when selected correlation terms were added on such that irregular behaviour was avoided.



n refers to the number of correlation terms used.

• refers to the Kohn scattering length, a_K .

+ refers to the singlet effective charge, $^1Z_{eff}$.

TABLE 2

Values of the linear parameters of the scattering wavefunction, F, for the PE case of the o-Ps-He system using the one parameter Hylleraas He ground state wavefunction when selected correlation terms were added on such that irregular behaviour was ignored.

n	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
Term																						
a_K	1.75	1.75	1.74	1.73	1.62	1.58	1.50	1.38	1.21	1.13	1.11	1.08	1.06	1.03	1.00	1.00	1.00	1.00	0.99	0.99	0.99	0.99
a_t	1.77	1.77	1.77	1.75	1.64	1.65	1.55	1.41	1.32	1.25	1.22	1.20	1.19	1.17	1.16	1.16	1.16	1.17	1.14	1.14	1.13	1.13
f_1	-.10	-.39	-.42	-.38	-.63	-.48	-.36	0.12	0.63	0.87	0.93	0.99	0.95	1.0	1.1	1.2	1.2	1.2	1.1	1.0	1.0	1.1
f_2	0.31	0.36	0.39	0.37	0.23	0.24	0.46	0.72	0.71	0.82	0.85	0.88	0.76	0.76	0.75	0.77	0.77	0.77	0.74	0.69	0.68	0.69
$10^2 f_3$	-0.8	-4	-5	-5	-3	-6	-5	-5	-10	-12	-12	-13	-12	-13	-13	-14	-14	-14	-12	-11	-11	-11
(0,0,0)	0	-.06	-.34	-.07	-1.6	-3.5	-7.2	-9.5	-12	-13	-13	-14	-16	-16	-17	-17	-17	-17	-17	-17	-17	-17
(0,0,1)	0	0	0.09	-.11	-.48	-.83	-1.2	-2.1	-3.8	-4.2	-4.5	-4.2	-4.3	-5.0	-4.8	-4.9	-4.9	-5.0	-5.2	-5.1	-5.3	-5.3
(0,0,2)	0	0	0	0.02	0.03	0.02	0.02	-.06	-.16	-.31	-.31	-.46	-.50	-.45	-.70	-.70	-.71	-.71	-.68	-.70	-.62	-.66
(0,1,0)	0	0	0	0	1.3	1.7	2.8	2.3	1.5	1.1	1.0	1.4	1.9	1.7	1.5	1.4	1.4	1.4	1.6	1.8	1.7	1.6
(1,0,0)	0	0	0	0	0	0.51	1.0	1.5	2.2	2.4	2.3	2.3	2.6	2.7	2.9	2.9	2.9	3.0	3.1	3.0	3.0	3.0
(0,3,0)	0	0	0	0	0	0	-.15	-.36	-.23	-.23	-.24	-.20	-.15	-.13	-.13	-.14	-.14	-.13	-.12	-.12	-.12	-.12
(0,1,1)	0	0	0	0	0	0	0	0.56	1.9	2.6	2.7	2.7	2.6	3.0	3.3	3.4	3.4	3.4	3.5	3.5	3.6	3.6
(0,2,1)	0	0	0	0	0	0	0	0	-.33	-.49	-.51	-.63	-.66	-.75	-.78	-.78	-.78	-.80	-.81	-.79	-.79	-.79
$10^2(3,1,1)$	0	0	0	0	0	0	0	0	0	0.01	0.03	0.03	0.07	0.08	0.08	0.03	0.08	0.09	2	2	2	2
$10^3(0,1,4)$	0	0	0	0	0	0	0	0	0	0	-0.1	-0.3	-0.5	-0.2	-0.1	-0.9	-1	-3	-6	-7	-7	-7
(0,1,2)	0	0	0	0	0	0	0	0	0	0	0	0.07	0.12	0.09	0.07	0.06	0.06	0.07	0.13	0.14	0.09	0.07
$10^2(3,1,0)$	0	0	0	0	0	0	0	0	0	0	0	0	-0.4	-0.4	-0.5	-0.4	-0.4	-0.4	0.1	0.1	0.04	0.05
$10^3(0,0,4)$	0	0	0	0	0	0	0	0	0	0	0	0	0	-0.8	-2	-2	-2	-2	-2	-2	-2	-3
$10^2(0,0,3)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.03	0.03	0.03	0.03	0.03	0.02	0.01	0.02
$10^2(1,1,3)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.1	0.2	1	2	2	2	2
$10^2(2,1,2)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-0.1	-1	-3	-3	-3	-3
$10^3(4,1,0)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-4	-5	-4	-4
(1,1,1)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-0.1	-.08	-.07	-.08
$10^3(1,2,1)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-7	-7	-6
$10^3(0,1,3)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	8
$10^5(0,0,5)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3

Here $f_i = \sigma^i e^{-0.7\sigma}$ and $(h,q,m) = e^{0.2|\vec{r}-\vec{r}_p|} e^{-1.2r} e^{-0.1r_p} |\vec{r}-\vec{r}_p|^m r^q r_p^h$

n refers to the number of correlation terms that are used.

TABLE 3

Values of the linear parameters of the scattering wavefunction, F, for the IE case of the o-Ps-He system using the one parameter Hylleraas He ground state wavefunction when selected correlation terms were added on such that irregular behaviour was ignored.

n	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Term																					
a_K	1.88	1.85	1.82	1.81	1.81	1.73	1.71	1.66	1.60	1.53	1.52	1.22	1.21	1.17	1.13	1.03	1.01	0.99	0.98	0.98	0.98
a_t	1.89	1.86	1.84	1.83	1.83	1.78	1.74	1.73	1.68	1.60	1.59	1.16	1.15	1.06	0.98	0.96	0.95	0.94	0.96	0.96	0.96
f_1	-.42	-.43	-.49	-.46	-.47	-.59	-.71	-.64	-.64	-.61	-.75	-.94	-.98	-1.3	-1.4	-1.1	-1.1	-1.3	-1.2	-1.2	-1.2
$10^2 f_2$	34	27	35	34	31	23	17	8	7	0.01	-6	-74	-78	-88	-86	-76	-90	-120	-93	-94	-95
f_3	-.04	-.02	-.04	-.04	-.04	-.06	-.04	-.05	-.06	-.07	-.07	0.09	0.10	0.14	0.16	0.09	0.11	0.15	0.09	0.09	0.09
(0,0,0)	0	0.56	-.02	0.12	0.18	0.60	1.6	0.90	1.4	6.1	6.4	21	22	22	24	35	34	39	36	36	36
(0,0,1)	0	0	0.19	0.10	0.09	0.45	0.62	0.39	0.37	1.1	1.6	4.6	4.7	4.8	5.5	8.5	8.6	9.6	9.0	9.2	9.3
10^2(0,0,3)	0	0	0	0.1	0.1	1	1	1	3	4	4	7	8	9	6	6	6	6	6	7	7
10^2(0,3,0)	0	0	0	0	1	10	12	17	20	31	36	1	1	0.4	-4	-12	-9	3	1	1	1
(0,1,2)	0	0	0	0	0	-.05	-.05	-.05	-.09	-.11	-.08	-.13	-.12	-.05	0.09	0.12	0.16	0.21	0.16	0.17	0.16
(1,0,0)	0	0	0	0	0	0	-.31	0.13	0.12	-.56	-.71	-3.1	-3.2	-3.1	-3.7	-6.7	-6.4	-7.5	-6.6	-6.7	-6.7
10^3(3,1,0)	0	0	0	0	0	0	0	-2	-9	-.05	-0.5	1	1	6	10	10	20	20	20	20	20
10^3(1,0,2)	0	0	0	0	0	0	0	0	-1	-1	-1	-3	-4	-4	-1	-2	-6	-1	-1	-1	-1
(0,1,0)	0	0	0	0	0	0	0	0	0	-1.6	-1.1	-8.1	-8.2	-8.3	-8.3	-14	-14	-15	-14	-14	-14
(0,1,1)	0	0	0	0	0	0	0	0	0	0	-.36	-1.0	-1.0	-.99	-1.5	-2.3	-2.7	-3.2	-2.8	-2.8	-2.9
(0,2,0)	0	0	0	0	0	0	0	0	0	0	0	3.3	3.3	3.6	3.8	4.8	4.8	5.1	4.3	4.3	4.3
10^5(3,0,2)	0	0	0	0	0	0	0	0	0	0	0	0	3	1	-4	-3	-7	-7	-8	-7	-7
(1,1,1)	0	0	0	0	0	0	0	0	0	0	0	0	0	-.14	-.14	-.26	-.16	-.20	-.19	-.18	-.18
(1,1,2)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-.01	-.01	-.02	-.02	-.01	-.02	-.02
(1,1,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.4	1.7	2.0	1.5	1.6	1.6
(2,1,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-.16	-.18	-.16	-.17	-.17
10^3(2,3,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2	-3	-3	-3
(1,2,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.15	0.15	0.15
10^4(0,0,2)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-.06	-.06
10^4(0,1,3)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6

Here $f_i = \sigma^i e^{-0.7\sigma}$ and $(h,q,m) = e^{0.2|\vec{r}-\vec{r}_p|} e^{-1.2r} e^{-0.1r_p} |\vec{r}-\vec{r}_p|^m r^q r_p^h$

n refers to the number of correlation terms that are used.

It has been standard procedure to give the results for the integer values of N as given in Table 4. Here the irregular behaviour starts to occur after N=1 for the PE and IE cases. A possible approach is to consider that the results at N=1 are reasonable. That is, before any irregular behaviour starts to occur. Here a_t=1.67a_o, a_K=1.6a_o with $^1Z_{eff}$=0.0599 for the PE case; a_K=1.816a_o, a_t=1.818a_o with $^1Z_{eff}$=0.0375 for the IE case.

4.3 o-Ps-He System Using Hartree-Fock Type He Wavefunction

In the static approximation it was found that the scattering length values were not sensitive to small changes of the non-linear parameter, δ, as in the Hylleraas situation. Again, convergence was reached after three terms and the results using δ = 0.9 are given in Table 5. These results are quite close to the values obtained for the IE case in the Hylleraas situation. Also the difference between the PE and IE values is much less than those obtained for the Hylleraas situation.

On adding 10 correlation terms to the wavefunction, the dependence of a_K on the non-linear parameters was found to be very similar to the Hylleraas situation. A suitable choice was found to be β = 0.2, γ = 1.3, η = 0.1 (using δ = 0.9). Again, more correlation terms were added to the wavefunction up to N = 5 (that is, 56 terms). It was found regardless of the order in which the

TABLE 4

Results for o-Ps-He system using one parameter Hylleraas He ground state wavefunction when the correlation terms were added on such that $h_j + q_j + m_j \leq N$.

(a) PE case

N	a_K	a_t	Z
0	1.754	1.775	0.0407
1	1.600	1.670	0.0599
2	2.768	2.813	0.0282
3	1.869	1.524	0.0544
4	2.096	1.996	0.0207
5	2.339	2.275	0.0114

(b) IE case

N	a_K	a_t	Z
0	1.857	1.863	0.0376
1	1.816	1.818	0.0375
2	0.7938	0.8654	0.147
3	1.761	1.842	0.0378
4	5.550	3.171	0.0263
5	3.180	2.158	0.0126

TABLE 5

Static Results for o-Ps-He scattering using a three parameter Hartree-Fock type ground state He wavefunction.

$\delta = 0.9$

(a) PE case

ℓ	a_K	a_t	Z
0	1.979	1.710	0.0412
1	1.910	2.050	0.0347
2	1.899	1.888	0.0336
3	1.899	1.885	0.0336

(b) IE case

ℓ	a_K	a_t	Z
0	1.988	1.725	0.0408
1	1.917	2.057	0.0344
2	1.907	1.896	0.0333
3	1.907	1.892	0.0333

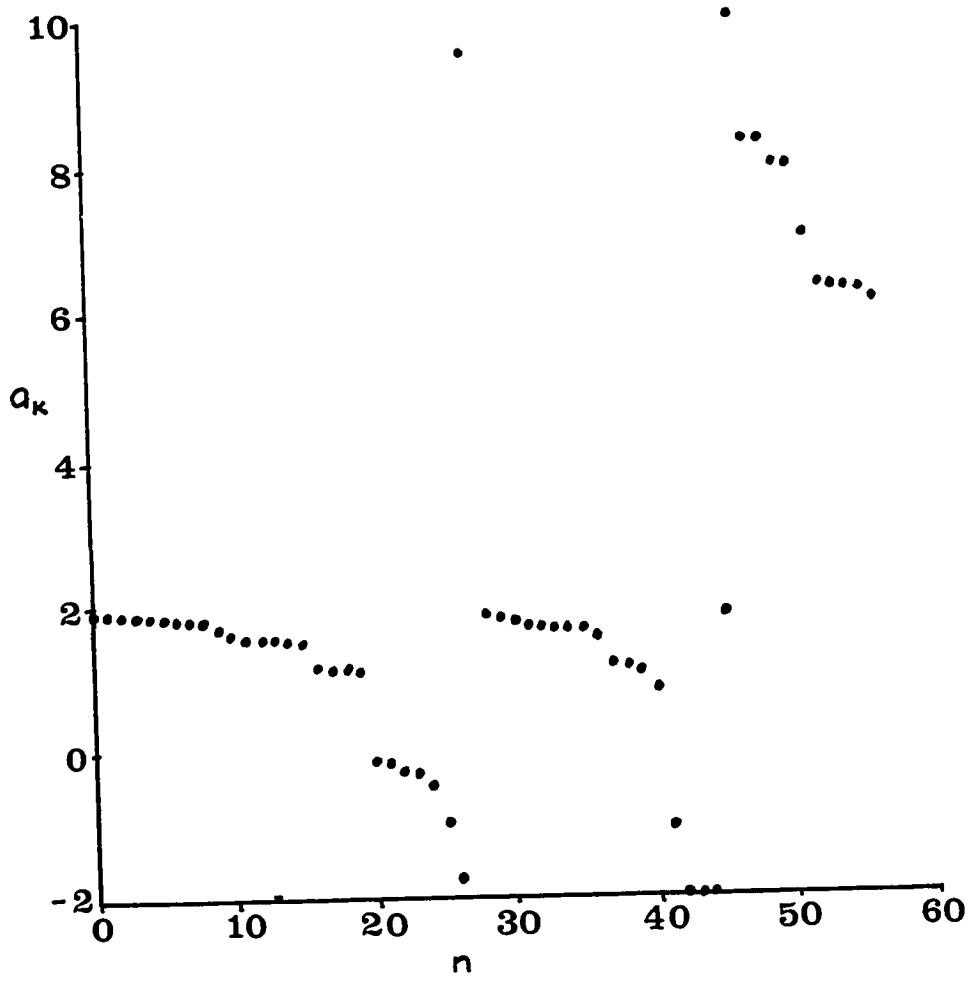
correlation terms were added the value of a_K always decreased at first. Irregular behaviour of a_K first appeared for larger numbers of correlation terms than in the Hylleraas situation as seen in Figures 5 and 6. This apparently better behaviour of the Hartree Fock type wavefunction was reported by Houston (1973b) in the e^+-He system.

Applying the reasoning given in the Hylleraas case, it was found that by rearranging the order in which the correlation terms were added the irregularities did not appear until the number of correlation terms was much larger. By this stage a_K appeared to have converged. This is shown in Figures 7 and 8 and is reflected to some extent by the small changes in the coefficients listed in Tables 6 and 7. For the PE case $a_K = 0.9651a_o$ with $a_t = 1.048a_o$ and $^1Z_{eff} = 0.127$; while for the IE case $a_K = 0.9764a_o$ with $a_t = 0.9766a_o$ and $^1Z_{eff} = 0.118$.

Using the variants of Peterkop and Rabik (1971) produced similar behaviour in the scattering length results. With the same correlation terms indicated in Tables 6 and 7 little change in the values of a_K from those given in the PE and IE cases was found. Here variant 2 gave $a_K = 0.9449a_o$, $a_t = 1.417a_o$ with $^1Z_{eff} = 0.132$; variant 3 gave $a_K = 1.070a_o$, $a_t = 1.198a_o$ with $^1Z_{eff} = 0.101$; variant 4 gave $a_K = 1.034a_o$, $a_t = 1.160a_o$ with $^1Z_{eff} = 0.107$. The convergence behaviour was similar to those shown in Figures 7 and 8. Note that

Figure 5

Results for the PE case of the o-Ps-He system using a three parameter Hartree-Fock type He ground state wavefunction when the correlation terms were added on such that $h_j + q_j + m_j \leq N$.

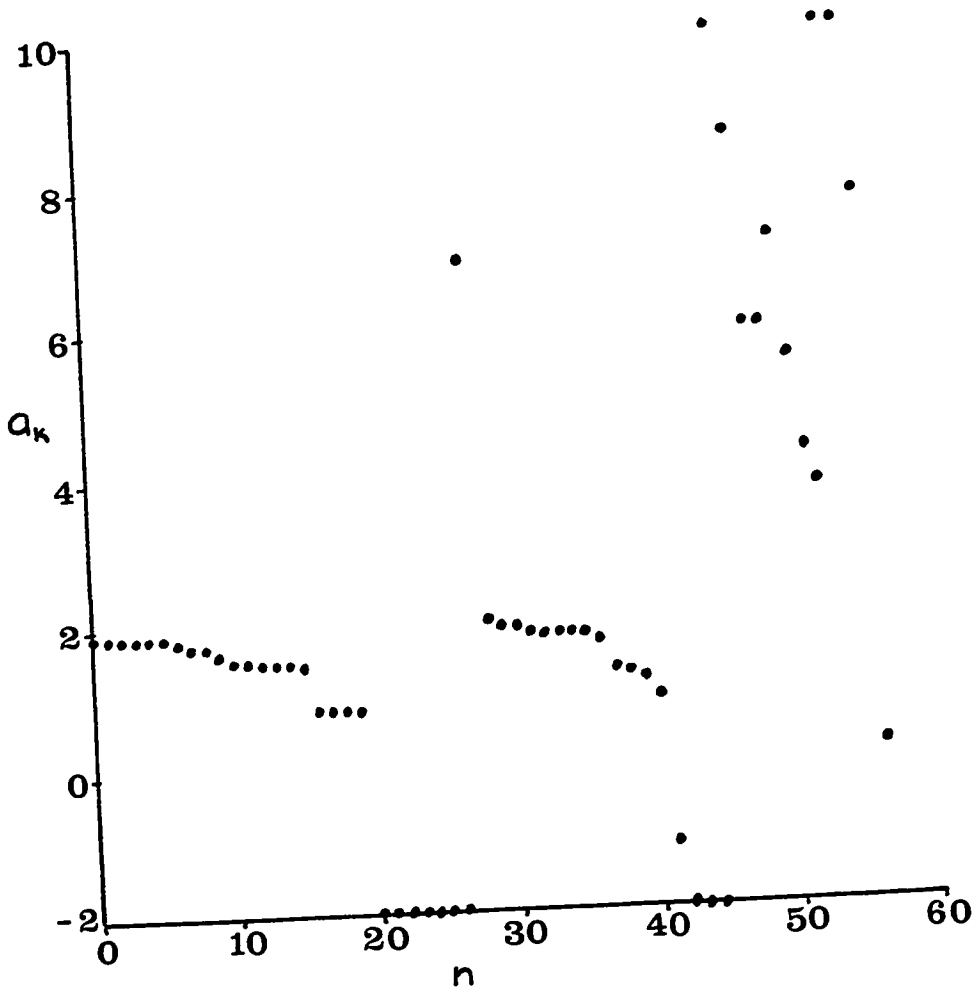


• refers to the Kohn scattering length, a_K.

n refers to the number of correlation terms used.

Figure 6

Results for the IE case of the o-Ps-He system using a three parameter Hartree-Fock type He ground state wavefunction when the correlation terms were added on such that $h_j + q_j + m_j \leq N$.

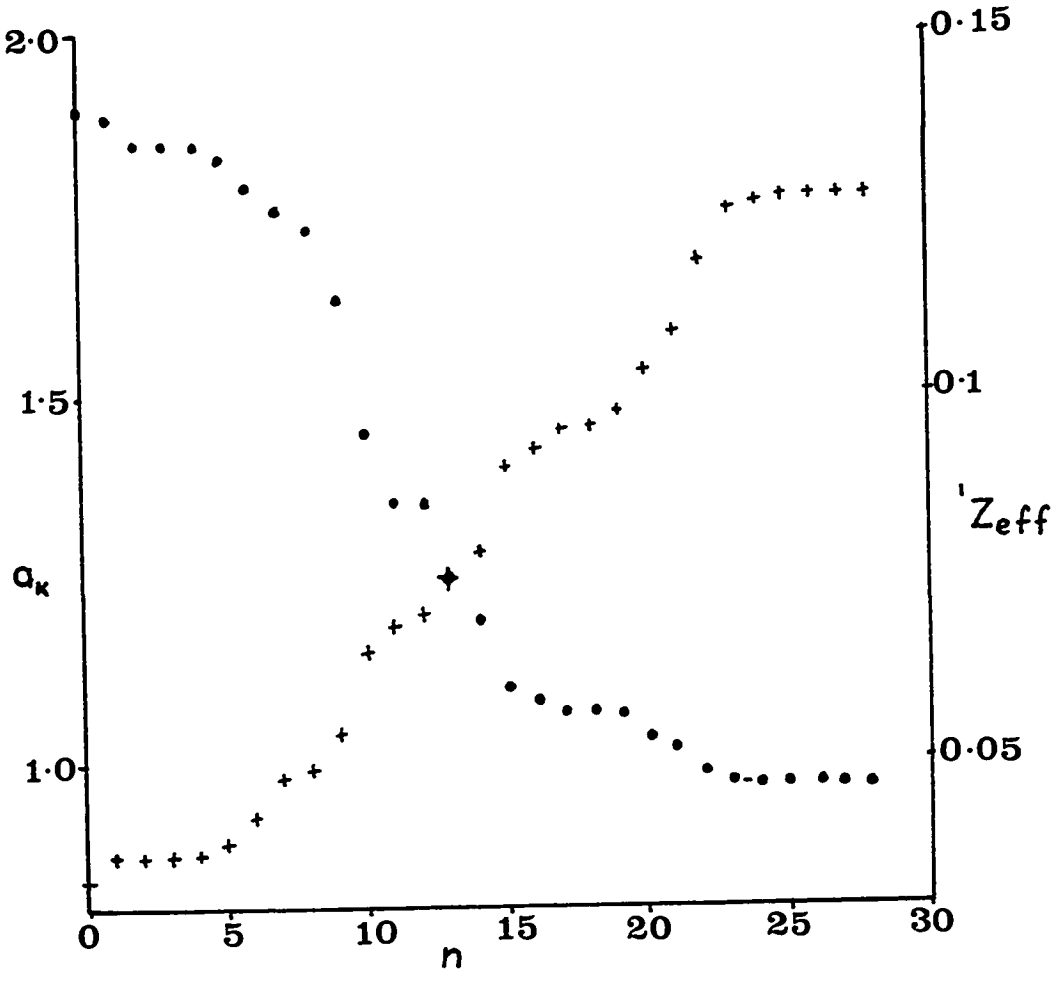


• refers to the Kohn scattering length, a_K.

n refers to the number of correlation terms used.

Figure 7

Results for the PE case of the o-Ps-He system using a three parameter Hartree-Fock type He ground state wavefunction when selected correlation terms were added on such that irregular behaviour was avoided.



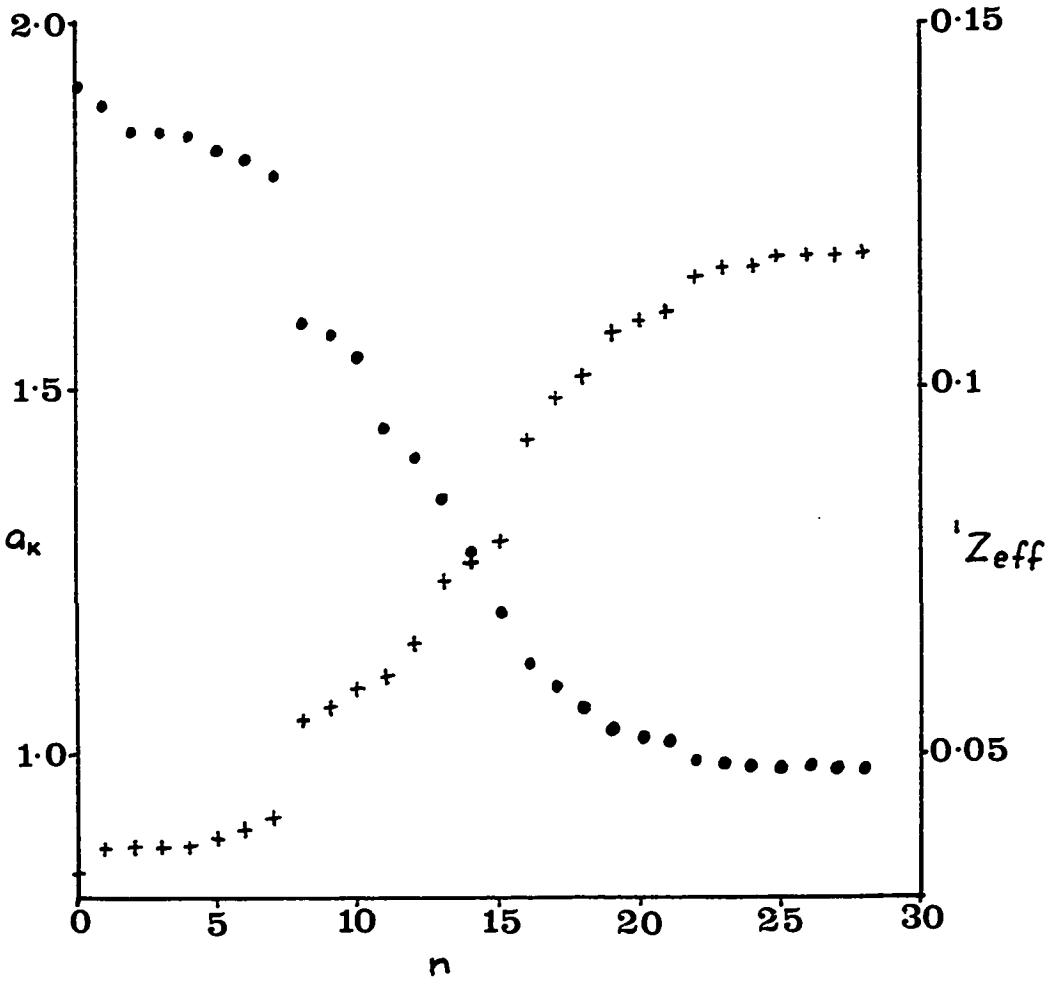
n refers to the number of correlation terms used.

• refers to the Kohn scattering length, a_K .

+ refers to the singlet effective charge, $^1Z_{eff}$.

Figure 8

Results for the IE case of the o-Ps-He system using a three parameter Hartree-Fock type He ground state wavefunction when selected correlation terms were added on such that irregular behaviour was avoided.



n refers to the number of correlation terms used.

• refers to the Kohn scattering length, a_K .

+ refers to the singlet effective charge, $^1Z_{eff}$.

TABLE 6

Values of the linear parameters of the scattering wavefunction, F, for the PE case of the o-Ps-He system using a three parameter Hartree-Fock type He ground state wavefunction when selected correlation terms were added on such that irregular behaviour was ignored.

n	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
Term																													
$10^2 a_K$	189	188	184	184	184	182	178	175	173	163	145	135	134	124	119	110	108	106	106	106	103	101	98	97	96	96	96	96	96
$10^2 a_t$	189	187	183	183	182	180	177	176	175	161	145	146	145	134	126	117	116	114	114	115	112	111	108	106	106	105	104	104	104
$10 f_1$	-8	-8	-8	-8	-8	-8	-8	-8	-9	-13	-15	-16	-16	-19	-19	-24	-22	-23	-23	-24	-25	-26	-29	-31	-31	-32	-32	-32	-32
$10 f_2$	2.5	1.9	2.8	2.8	2.6	2.2	0.6	-1	-.5	-6	-3	-12	-13	-27	-28	-39	-39	-41	-41	-43	-47	-51	-57	-59	-60	-61	-61	-61	-61
$10^2 f_3$	-.1	0.6	-.7	-.7	1	2	-.9	-2	-6	11	-3	0.7	1	27	33	51	50	54	53	54	63	69	79	82	84	86	87	86	86
(0,0,0)	0	.54	-.1	-.1	.59	1.0	5.3	7.5	7.4	3.9	4.7	13	13	20	19	31	27	28	28	29	31	32	34	30	30	29	30	31	31
(0,0,1)	0	0	.24	.23	.38	.08	.69	1.0	1.0	.03	1.7	4.1	3.9	5.1	4.7	6.9	5.9	5.7	5.7	6.1	7.1	7.5	7.1	6.1	6.1	5.8	6.0	6.0	6.0
(0,1,0)	0	0	0	.002	-.1	-.1	-2	-3	-4	-1	-.7	-5	-5	-8	-6	-11	-10	-10	-10	-10	-11	-12	-13	-11	-11	-10	-11	-11	-11
(1,0,0)	0	0	0	0	-.2	-.2	-.9	-1	-.7	1.1	1.2	-1	-1	-3	-3	-6	-4	-4	-4	-4	-4	-2	-2	2.2	2.8	3.0	2.3	2.0	1.7
(0,0,2)	0	0	0	0	0	.04	.04	.07	.19	.39	.71	.79	.86	1.2	.92	1.0	.85	.98	1.0	1.0	1.1	1.0	1.6	1.7	1.7	1.6	1.6	1.6	1.7
(0,2,0)	0	0	0	0	0	0	.72	1.4	1.6	1.7	1.5	3.6	3.7	6.7	6.6	6.6	9.1	8.9	9.3	9.3	9.6	10	11	12	12	12	12	12	12
(0,2,1)	0	0	0	0	0	0	0	-.07	-.1	.02	.31	.79	.80	1.0	1.1	1.3	1.3	1.3	1.3	1.3	1.4	1.5	1.6	1.6	1.7	1.7	1.7	1.7	1.7
(1,0,1)	0	0	0	0	0	0	0	0	-.2	-.3	-.6	-.6	-.6	-.8	-.2	-.3	0.4	.47	.43	.43	.35	.71	1.0	1.5	1.6	1.9	1.8	1.8	1.7
(1,1,0)	0	0	0	0	0	0	0	0	0	-.9	-.5	1.4	1.4	2.5	2.2	3.3	3.1	3.1	3.2	3.3	3.8	4.1	4.5	3.2	3.0	2.9	3.1	3.1	3.1
(0,1,1)	0	0	0	0	0	0	0	0	0	0	-2	-3	-3	-5	-5	-6	-6	-6	-6	-6	-7	-8	-8	-8	-9	-9	-9	-9	-8
(1,2,0)	0	0	0	0	0	0	0	0	0	0	0	-.6	-.6	-1	-1	-2	-2	-2	-2	-2	-2	-3	-3	-3	-3	-3	-3	-3	-3
10^2(0,0,3)	0	0	0	0	0	0	0	0	0	0	0	0	-.5	-1	3	10	13	13	12	12	11	16	8	10	9	10	13	14	11
(2,2,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	.03	.04	.05	.05	.05	.05	.05	.06	.07	.07	.04	.04	.04	.04	.04	.04
10^2(1,0,2)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-6	-18	-23	-25	-24	-25	-25	-34	-42	-50	-50	-52	-61	-62	-57
(3,0,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.04	.07	.07	.07	.08	.10	.22	.32	.37	.39	.39	.34	.32	.28
10(2,0,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-6	-6	-6	-7	-9	-18	-26	-35	-37	-38	-36	-35	-33
10^4(1,0,4)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.3	-.1	-.1	-.6	3	6	8	8	8	8	8	10
10^4(0,0,5)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.5	.4	1	-1	-6	-7	-8	-8	-7	-8	-10
(0,1,2)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.01	.10	.13	.17	.16	.21	.23	.24	.24	.23
10^4(1,1,3)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-4	-5	-5	-5	-3	-5	-5	-6	-6
10^3(4,0,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-4	-8	-9	-9	-9	-9	-7	-5
10^2(0,0,4)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.9	1	1	1	1	1
(2,1,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.15	.18	.24	.24	.24	.24
10^3(1,1,2)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-8	-1	-.2	.8	2
10^2(1,1,1)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-14	-15	-16	-18
(2,0,1)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.11	.11	.11
10^4(5,0,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-.3	-1
10^3(1,0,2)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-7

Here $f_1 = \sigma^1 e^{-0.9\sigma}$ and $(h,q,m) = e^{0.2|\vec{r}-\vec{r}_p|}\ e^{-1\cdot\vec{3}r}\ e^{-0.1r_p}\ |\vec{r}-\vec{r}_p|^{m} r_{12}^{q}\ r_p^{h}$

n refers to the number of correlation terms that are used.

TABLE 7

Values of the linear parameters of the scattering wavefunction, F, for the IE case of the o-Ps-He system using a three parameter Hartree-Fock type He ground state wavefunction when selected correlation terms were added on such that irregular behaviour was ignored.

n	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
Term																													
$10^2 a_K$	190	188	184	184	184	182	181	179	158	157	154	144	140	134	128	119	111	108	105	103	101	101	98	98	98	98	97	97	97
$10^2 a_t$	187	187	183	183	181	179	178	176	153	151	151	142	143	139	126	111	110	108	106	106	103	103	100	99	99	98	97	97	97
$10 f_1$	-8	-8	-9	-9	-9	-8	-9	-8	-10	-10	-11	-12	-10	-11	-15	-15	-21	-22	-24	-25	-26	-27	-29	-30	-30	-31	-31	-31	-31
$10 f_1$	2.5	1.9	2.8	2.9	2.6	2.3	2.1	2.1	.6	.8	.4	2.8	3.4	.2	-7	-10	-17	-19	-23	-26	-28	-28	-32	-32	-32	-34	-34	-34	-33
$10^2 f_2$	0.6	0.8	-.6	-.7	1	2	3	2	2	1	0.1	-7	-15	-18	3	14	19	20	27	28	33	33	39	40	40	44	43	44	43
$10^2 f_3$																													
10(0,0,0)	0	5.8	-.5	0.2	8.1	12	5.9	5.9	36	35	22	12	-21	49	0.1	-12	46	43	37	8.3	-15	-10	1.4	3.7	9.0	3.3	12	10	7.3
10(0,0,1)	0	0	2.5	2.6	4.3	1.3	1.6	-2	7.7	7.0	7.5	15	9.9	20	0.9	-2	9.5	5.1	4.3	3.6	-5	-3	-10	-10	-8	-8	-7	-7	-8
10(0,1,0)	0	0	0	-.6	-2	-2	3.2	1.9	8.9	11	16	12	17	16	14	36	23	26	39	43	52	50	51	52	49	55	52	52	52
(1,0,0)	0	0	0	0	-.2	-.3	-.2	-.1	-.7	-.5	-.2	1.3	3.3	1.7	4.9	4.5	3.6	4.1	6.1	9.9	13	13	12	12	12	12	12	12	12
(0,0,2)	0	0	0	0	0	.04	.06	.11	.28	.38	.38	.64	.48	.63	.83	.41	.80	.71	.89	.87	1.0	1.0	1.0	1.0	.97	.87	1.0	1.1	1.1
10(0,1,1)	0	0	0	0	0	0	-1	-.4	-11	-13	-15	-18	-21	-20	-18	-19	-31	-33	-39	-43	-45	-47	-45	-46	-46	-48	-48	-48	-47
10^2(1,1,2)	0	0	0	0	0	0	0	-.1	-.3	-.2	.1	-.2	-.4	-.2	-.6	-1	-1	-1	-1	-.9	-.9	-1	2	1	1	1	.6	.6	.9
(0,2,1)	0	0	0	0	0	0	0	0	.31	.33	.37	.46	.51	.38	.43	.51	.84	.86	.99	1.0	1.0	1.0	1.1	1.1	1.1	1.1	1.1	1.1	1.1
10^2(1,0,2)	0	0	0	0	0	0	0	0	0	-1	-.9	.5	.7	.09	-1	-9	-13	-21	-25	-33	-47	-47	-62	-68	-67	-70	-63	-57	-58
10^2(3,1,0)	0	0	0	0	0	0	0	0	0	0	-.3	-.1	.1	.1	.8	1	2	2	1	1	.9	1	1	1	1	1	1	1	1
10(1,0,1)	0	0	0	0	0	0	0	0	0	0	0	-5	.1	-2	-.1	7.1	5.7	11	13	18	24	23	32	33	32	35	32	31	31
10(2,0,0)	0	0	0	0	0	0	0	0	0	0	0	0	-5	-3	-6	-6	-6	-8	-11	-23	-34	-33	-36	-37	-35	-38	-35	-37	-38
(0,2,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	1.5	1.7	1.6	2.6	2.9	3.5	3.9	4.2	4.3	4.6	4.7	4.7	4.8	4.8	4.8	4.8
10(1,1,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-12	-17	-15	-16	-27	-32	-39	-38	-38	-39	-38	-39	-38	-38	-39
(0,0,3)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.07	.08	.12	.13	.17	.21	.21	.26	.29	.30	.31	.25	.21	.21
10^2(2,2,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-4	-4	-6	-8	-8	-9	-9	-9	-9	-9	-9	-9	-9
10^2(4,0,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.1	.2	.1	-.5	-.6	-.9	-1	-1	-1	-2	-2	-2
(2,1,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.22	.33	.46	.40	.49	.48	.48	.52	.51	.51	.55
(3,0,0)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.09	.20	.20	.20	.23	.21	.23	.21	.22	.23
10(3,0,1)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.07	.07	.1	.1	.2	.2	.4	.5	.5
10^2(1,1,1)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	-27	-22	-25	-29	-30	-32	-34
10^3(1,1,3)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	-1	-1	-.8	-.8	-1
10^4(0,0,5)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-.4	-.1	-.2	-.7	-3	-3
10^2(2,0,2)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-.7	-.6	-2	-3	-3
(0,1,2)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	.08	.10	.11	.10
10^3(0,0,4)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	9	9
10^4(1,0,4)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	3
10^4(3,1,1)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2

Here $f_1 = \sigma^1 e^{-0.9\sigma}$ and $(h,q,m) = e^{0.2|\vec{r}-\vec{r}_p|} e^{-1.3r} e^{-0.1r_p} |\vec{r}-\vec{r}_p|^m r^q r_p^h$

n refers to the number of correlation terms that are used.

variant 1 corresponds to the IE case.

Taking the IE case as an example, it was found that if the correlation terms were added on in "reverse" order, that is, starting with the term in r_p^5 and working backwards, the above approach gave a converged value of $a_K = 0.9721a_o$, $a_t = 1.090a_o$, and $^1Z_{eff} = 0.076$ after 15 terms. The comparatively low value of $^1Z_{eff}$ is attributed to the exclusion of low powers of the variables r_1, ρ_1 and r_p in the wavefunction. Similarly, it was found that beginning with any of the first 56 correlation terms and adding more terms on up to about 20 terms gave a converged value of $a_K \simeq 1.0a_o$ with $^1Z_{eff}$ ranging from 0.08 to 0.12. These results tend to support the estimate that $a_K \simeq 1.0a_o$ with $^1Z_{eff} \simeq 0.12$.

In the other appreach considered the value of a_K in the flat portions of the curves of Figures 5 and 6 is determined. Here the estimates are $a_K = 1.08a_o$, $a_t = 1.17a_o$ with $^1Z_{eff} = 0.097$ for the PE case; $a_K = 1.40a_o$, $a_t = 1.37a_o$ with $^1Z_{eff} = 0.076$ for the IE case.

No significant change in the results appeared when the Hulthén method was used.

Listing the results for integer values of N is done in Table 8. Here the irregular behaviour occurs after N = 2 for both the PE and IE cases. As in the Hylleraas situation, a possible approach is to consider the values at the last N before any irregularities in a_K occur. At

TABLE 8

Results for o-Ps-He system using a three parameter Hartree-Fock type ground state He wavefunction when the correlation terms were added on such that $h_j + q_j + m_j \leq N$.

(a) PE case

N	a_K	a_t	Z
0	1.881	1.870	0.0369
1	1.843	1.822	0.0373
2	1.574	1.596	0.0615
3	-0.1171	-0.01976	0.320
4	1.654	1.709	0.0648
5	6.063	5.509	1.36

(b) IE case

N	a_K	a_t	Z
0	1.886	1.874	0.0369
1	1.843	1.819	0.0370
2	1.492	1.519	0.0676
3	-2.169	-1.872	0.955
4	1.764	1.804	0.0603
5	0.1242	-1.044	0.213

$N = 2$, $a_t = 1.596a_o$, $a_K = 1.574a_o$ with $^1Z_{eff} = 0.0615$ for the PE case; $a_K = 1.492a_o$, $a_t = 1.519a_o$ with $^1Z_{eff} = 0.0676$ for the IE case.

4.4 Ps-H System

The results given in this section are listed under two cases corresponding to the symmetry property of the wavefunction, namely, the Antisymmetric and Symmetric cases. In the static approximation it was found that $\delta = 0.9$ gave the best results. More terms were needed for convergence compared to the o-Ps-He system. The results are given in Table 9. These results differ from those previously calculated by Fraser (1961). He obtained $a_+ = 13.4a_o$ and $a_- = 1.84a_o$. It is believed that the discrepancy is due to the use of insufficient integration points in the earlier work by Fraser. Using the appropriate expression developed by Fraser (1961) the total cross section and conversion cross section can be calculated. Here the total cross section, σ_t, is

$$\sigma_t = \pi(3(a_-)^2 + (a_+)^2)$$

and the conversion cross section, σ_p, is

$$\sigma_p = 0.25\pi(a_- - a_+)^2$$

where a_- and a_+ are the zero-energy scattering lengths for the Antisymmetric and Symmetric cases respectively. Taking $a_+ = 7.27a_o$ and $a_- = 2.48a_o$ gives $\sigma_t = 165\pi a_o^2$,

TABLE 9

Static Results for Ps-H scattering

$\delta = 0.9$

(a) Antisymmetric

ℓ	a_K	a_t
0	2.611	2.175
1	2.482	2.533
2	2.482	2.518
3	2.481	2.471
4	2.481	2.482

(b) Symmetric

ℓ	a_K	a_t
0	29.89	16.59
1	7.423	7.921
2	7.308	7.606
3	7.301	7.101
4	7.271	7.330
5	7.269	7.269

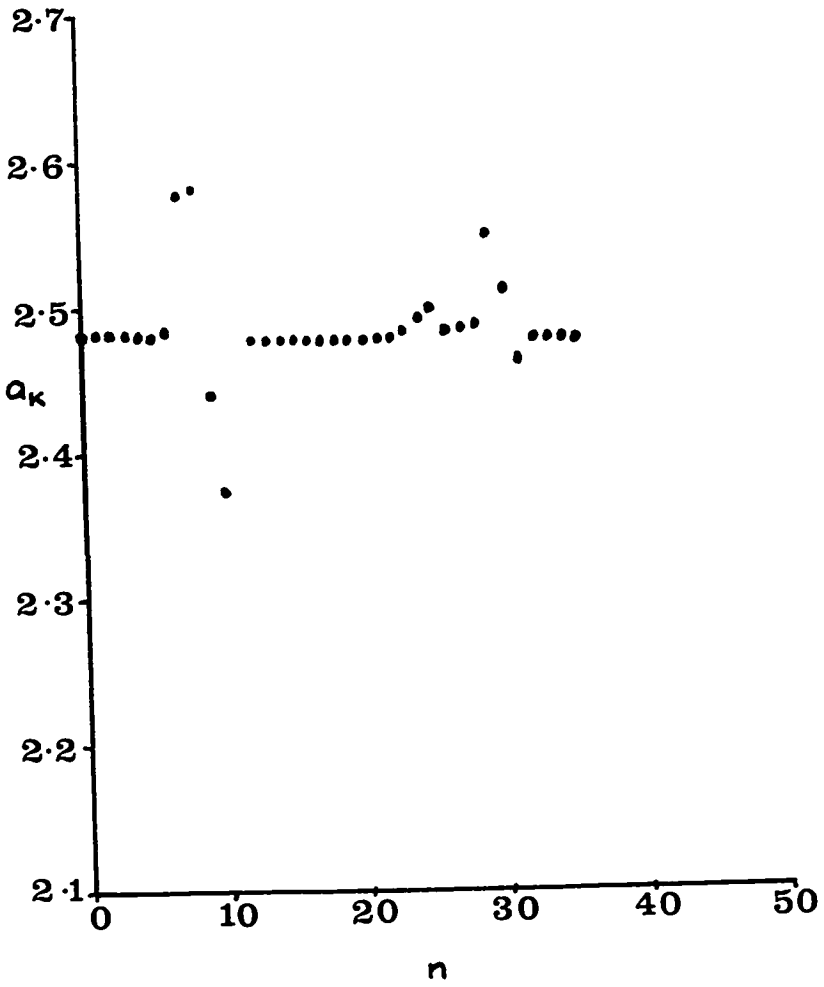
$\sigma_p = 5.74\pi a_o^2$ and $\sigma_p/\sigma_t = 0.035$.

After adding 10 correlation terms, a search was carried out to find suitable values for the non-linear parameters. In the Antisymmetric case it was found that a_K was insensitive to the choice of values given to β, γ and η. For the Symmetric case it was found that the values $\beta = 0.2$, $\gamma = 0.8$, $\eta = 0.3$ with $\delta = 0.5$ gave a reasonable change in the value of a_K. Keeping the non-linear parameters fixed at these values, more correlation terms were added up to 35 terms. As in the o-Ps-He system, irregularities occurred.

Since an exact target ground state wavefunction was used it is not clear why there should be irregular behaviour in the Antisymmetric case except if due to truncation errors (see Section 4.5). From Figure 9 the value of a_K appears to be converging to $a_K = 2.474a_o$. For the Symmetric case, the situation is quite obscure as given by Figure 10. This is due to the fact that since there is a composite projectile-target bound state, the normal Kohn method does not provide an upper bound on the exact scattering length. There appeared to be a downward trend in the value of a_K, as the number of correlation terms increased, to $a_K = 3.447a_o$ with $a_t = 3.456a_o$ (the values of a_K and a_t on adding 34 correlation terms). Bearing in mind that this interpretation of the results must be viewed with caution, these values give

Figure 9

Results for the Antisymmetric case of Ps-H when the correlation terms were added on such that $h_j + q_j + m_j \leq N$.

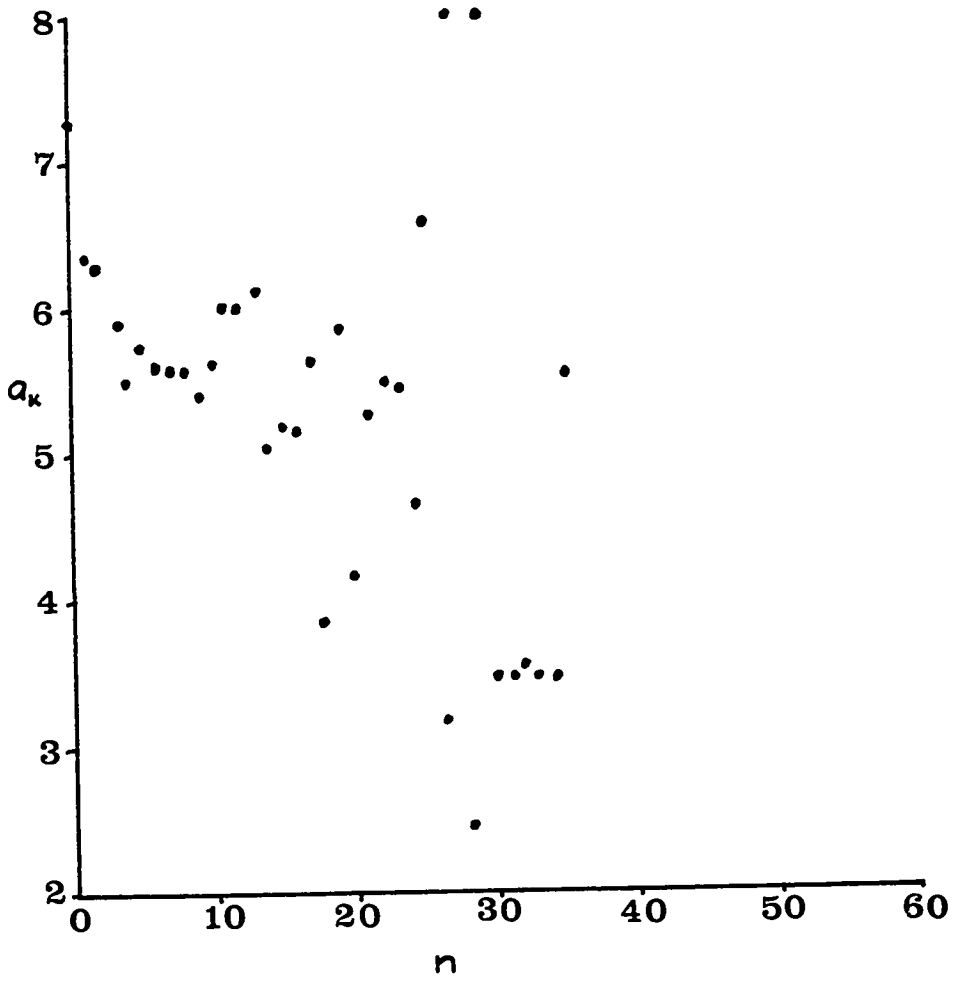


n refers to the number of correlation terms used.

• refers to the Kohn scattering length, a_K.

Figure 10

Results for the Symmetric case of Ps-H when the correlation terms were added on such that $h_j + q_j + m_j \leq N$.



• refers to the Kohn scattering length, a_K.

n refers to the number of correlation terms used.

$\sigma_t = 41.8\pi a_o$, $\sigma_p = 0.30\pi a_o$ and $\sigma_p/\sigma_t = 7.2 \times 10^{-3}$.

The results for integer values of N are listed in Table 10. Apart from the values at N = 2, there appears to be reasonable convergence in the Antisymmetric case. In the Symmetric case the situation is less obvious. It is difficult to know whether either the N = 3 result or the N = 4 result is irregular. Results for higher values of N would be needed to resolve this difficulty but were not obtained because of lack of time and money.

Recently, Houston and Drachman (1973) calculated the binding energy of PsH against dissociation into Ps and H. They obtained a value of 0.0497 rydbergs (0.672eV) as compared to the value of 0.0484 rydbergs determined by Lebeda and Schrader (1969). Now the binding energy is related to the scattering length by the formula (see, for example, Mott and Massey (1965)).

$$-1/a = -\kappa + \kappa^2 r_o/2 + \text{higher orders of } \kappa$$

with

$$E = \hbar^2\kappa^2/2m \quad .$$

Here E is the binding energy of the projectile-target, m is the mass of the projectile, κ is the projectile wave number, a is the zero-energy scattering length and r_o is the effective range parameter. This expansion is valid only for short range potentials.

In atomic units, $\hbar = 1$, with m = 1 in this case and E is in rydbergs. Using the value of E = 0.0497 rydbergs

TABLE 10

Results for the Ps-H system when the correlation terms were added on such that $h_j + q_j + m_j \leq N$.

(a) Antisymmetric

N	a_K	a_t
0	2.481	2.521
1	2.482	2.540
2	2.350	2.318
3	2.475	2.515
4	2.474	2.509

(b) Symmetric

N	a_K	a_t
0	6.381	5.155
1	5.499	4.706
2	5.355	4.403
3	4.187	4.470
4	5.579	5.428

and neglecting κ^2 and higher order terms

$$a = 1/\kappa = 3.17a_o \ .$$

Keeping the second order term and neglecting higher orders gives

$$r_o = 2(\kappa - 1/a)/\kappa^2 \ .$$

Using $a = 3.45a_o$ and $E = 0.0497$ rydbergs gives $r_o = 0.51a_o$. While there are no experimental results for comparison, the above results seem to be physically reasonable.

4.5 Effect Of Truncation Errors

A test was performed on the effect of truncation errors accumulating in solving the simultaneous equations that are generated from equations (3.21), (3.22). On changing the fourth or fifth significant digit by one in a random fashion, of the various matrix elements involved it was found that in general the third significant figure of the final results was altered.

An exception was the PE case in the Hartree Fock situation. Here the second significant figure of the final results was altered. Furthermore, in this particular case, when all of the matrix elements were changed by one in a random fashion in the third or fourth significant digit, irregular behaviour in the resulting a_K values occurred. This irregular behaviour in a_K appeared after 19 correlation terms were added to the trial wavefunction. It is interesting to note that the final results (that is, using the 28 selected terms) of $a_K = 0.9706a_o$, $a_t = 1.053a_o$ with

$^1Z_{eff}$ = 0.132 is quite close to the values obtained using the normal matrix elements. This suggests that the effect of truncation errors is not serious.

As a further test, the matrix elements F_{ij}, S_{ij} and K_{ij} were used in an eigenvalue calculation. It was found that the eigenvalues became meaningless after about 40 correlation terms were used. This suggests that the results using up to 40 correlation terms may be considered reliable.

4.6 Summary

Results have been given from applying the Kohn variational principle to the zero-energy scattering of o-Ps by a He and a H atom. In the static approximation good agreement was obtained with earlier results of Fraser and Kraidy (Fraser (1962), Fraser and Kraidy (1966), Fraser (1968b), Kraidy (1969, private communication)) for the o-Ps-He system using a single parameter Hylleraas ground state He wavefunction. It is interesting to note that the results obtained using a three parameter Hartree-Fock type ground state He wavefunction gave reasonable agreement with the IE case of the Hylleraas situation in the static approximation.

The introduction of correlation terms of the form given in equation (3.7) into the trial wavefunction produced a marked change in the numerical results for the o-Ps-He system. Here, irregular behaviour of a_K made an

accurate determination of the scattering length extremely difficult since the values of a_K do not necessarily represent an upper bound on the scattering length. The approaches used to determine the scattering length gave values ranging from $a_K = 2.33a_o$ to $a_K \simeq 1.0a_o$ with $^1Z_{eff} = 0.011$ to $^1Z_{eff} \simeq 0.12$ respectively.

For the o-Ps-H system the static results obtained differ from those previously calculated by Fraser (1961). The effect of the addition of correlation terms in the calculations was extremely different in the Antisymmetric and Symmetric cases respectively. A very small change in the scattering length value was observed in the Antisymmetric case. The final result being $a_K = 2.474a_o$.

Irregularities in the value of a_K for the Symmetric case prevented a reliable interpretation of the results. There appeared to be a significant decrease in the value of a_K. Using this interpretation gave an appreciable lowering of the cross sections from those that were determined by the static approximation.

CHAPTER 5

CONCLUSION

An extensive Kohn variational calculation on the zero-energy scattering of o-Ps by a He atom has been attempted. Using the static approximation, good agreement was obtained with the earlier results of Fraser and Kraidy (Fraser (1962), Fraser and Kraidy (1966), Fraser (1968b), Kraidy (1969), private communication)) who solved an integro-differential equation. This illustrates the reliability of the Kohn method as compared with another technique, namely, directly solving an integro-differential equation.

It became apparent during the course of the work that the Kohn method was not necessarily reliable when approximate ground state target wavefunctions were used. Considerable change in the results was produced by the inclusion of short-range correlation terms in the trial wavefunction. These terms could be interpreted as describing the distortion of the Ps atom and the formation of virtual excited states of Ps.

Also the exchange terms in the trial wavefunction allowed to some extent for the distortion of the helium atom. An improvement would be to include correlation terms that allowed for distortion of the helium atom

explicitly.

Irregular behaviour of the values of a_K occurred as the number of the correlation terms was increased. This behaviour was believed to be due to the use of an inexact He ground state wavefunction in the calculations. Attempts to determine an estimate of the scattering length had to be based on non-rigorous criteria. The results obtained varied from $a_K = 2.33a_o$ to $a_K \simeq 1.0a_o$ with ${}^1Z_{eff} \simeq 0.011$ and ${}^1Z_{eff} \simeq 0.12$ respectively. These findings demonstrate the difficulties encountered in using the Kohn variational method for systems in which an approximate ground state target wavefunction is used. No irregularities were observed in the static approximation calculations. But when correlation terms describing distortion of either the target or the projectile are introduced into the trial wavefunction, then the outcome of the Kohn results depends primarily on the nature of the approximate ground state target wavefunction used. Unfortunately, only two rather simple approximations to the ground state He wavefunction were used in the present calculations.

It is felt that in order to obtain better estimates of the scattering length, a, more accurate He ground state wavefunctions must be used such as the many-parameter Hylleraas type wavefunctions (Hylleraas (1929)). This difficulty in obtaining reliable estimates of a has been

encountered in other systems, notably, the e^--He and e^+-He systems (Houston (1973a, 1973b)). In particular, Houston and Moiseiwitsch (1968) calculated a_K for the e^+-He system using the three parameter Hartree-Fock type ground state wavefunction. They found a reasonable convergence up to 20 terms and seemed to have obtained a pseudo-upper bound on a. However, irregular behaviour of a_K started to occur after 22 terms (Houston (1973b). Nevertheless, the result of Houston and Moiseiwitsch supports the approach which assumed a_K initially tended to converge to the true scattering length as the correlation terms were added on.

The requirement of $a > 0$ is necessary for an overall repulsive interaction between the o-Ps atom and the He atom (De Benedetti (1964)). It is this repulsive interaction that is responsible for the formation of bubbles around o-Ps in liquid or very dense gaseous He (Ferrel (1956, 1957)). Furthermore, the investigations of Peterkop and Rabik (1971) indicate a convergence in the values of a_K to a value very close to the correct a, if the irregularities of a_K are ignored.

Perhaps, these observations favour the result of $a_K = (1.0 \pm 0.1)a_o$ with $^1Z_{eff} = 0.12 \pm 0.02$. Certainly, this result seems to be in better agreement with most experimental findings than previous theoretical results. However, Spektor and Paul (1973, to be published) measured the elastic cross section, σ, of o-Ps and He

and obtained $\sigma = (30.05 \pm 0.27)\pi a_o^2$. Since $\sigma = 4\pi a^2$, this value of σ corresponds to a value of $a = (2.74 \pm 0.13)a_o$ which is at variance with the findings given here.

A similar calculation was performed on the Ps-H system. Although, in the static approximation, quite a discrepancy in the results was found with those previously determined by Fraser (1961), it is believed that the static results presented here are more accurate. Very little change was observed in the value of a_K as the correlation terms were added to the trial wavefunction for the Antisymmetric case, the final result being $a_K = 2.474a_o$. An improvement on this value would involve including other correlation terms involving the atomic electron coordinate into the trial wavefunction. Such calculations become increasingly more difficult to carry out.

A reliable analysis of the results for the Symmetric case was prevented due to the occurence of irregular behaviour of the values of a_K. An interpretation, based on the observed trend of the values of a_K as the correlation terms were added on, gave $a_K = 3.447a_o$. Using this value gave $\sigma_t = 41.8\pi a_o^2$, $\sigma_p = 0.30\pi a_o^2$ and $\sigma_p/\sigma_t = 7.2\text{x}10^{-3}$. However, it must be remembered that these results must be viewed with caution. Undoubtedly, a reliable estimate could be determined by incorporating the procedure of Rosenberg et al (1960).

Additional Note

The experimental result of Spektor and Paul mentioned on the previous page has been revised. A more recent value known is that $\sigma \leq 12\pi a_o^2$ which gives $|a| \leq 1.73a_o$.

APPENDIX A

REDUCTION OF TYPICAL INTEGRALS

Consider the integral

$$P(a,b,r,t) = \int e^{-ar} e^{-b|\vec{r}-\vec{t}|} r^{-1} |\vec{r}-\vec{t}|^{-1} d\vec{r}$$

$$2\pi \int_0^{\infty} r^2 e^{-ar} r^{-1} dr \int_{-1}^{1} d\eta (r^2+t^2-2rt\eta)^{-\frac{1}{2}} e^{-b(r^2+t^2-2rt\eta)^{\frac{1}{2}}}$$

where $\eta = \dfrac{\vec{r} \cdot \vec{t}}{r\ t}$ .....(A.1)

Let $E=\int_{-1}^{1} d\eta (r^2+t^2-2rt\eta)^{-\frac{1}{2}} e^{-b(r^2+t^2-2rt\eta)^{\frac{1}{2}}}$, $p=t/r, \zeta = |\vec{r}-\vec{t}|$.

Then $\int_{-1}^{1} d\eta \rightarrow -\int_{r+t}^{|\vec{r}-\vec{t}|} (1/rt)\zeta d\zeta = (1/rt)\int_{|\vec{r}-\vec{t}|}^{r+t} \zeta d\zeta$

It is convenient to normalize the integration limits from +1 to -1 through a change of variable

$\xi = -1/p+\zeta/t$ for $p \leq 1$, $\xi = \zeta-p+\zeta/r$ for $p \geq 1$. In terms of this new variable, ξ,

$\eta = p/2-\xi-p\xi^2/2$, $|\vec{r}-\vec{t}| = (1+p\xi)$, $d\eta = -d\xi(1+p\xi)$ for $p \leq 1$;

$\eta = 1/2p-\xi-\xi^2/2p$, $|\vec{r}-\vec{t}| = r(p+\xi)$, $d\eta = -d\xi(1+\xi/p)$ for $p \geq 1$.

Thus

$$E=\int_{-1}^{1} d\xi r^{-1} e^{-br(1+p\xi)} = e^{-br}(e^{bt}-e^{-bt})/brt \text{ for } p \leq 1 .$$

$$E=\int_{-1}^{1} d\xi t^{-1} e^{-br(p+\xi)} = e^{-bt}(e^{br}-e^{-br})/brt \text{ for } p \geq 1 .$$

Hence $P = 2\pi\int_0^\infty re^{-ar}Edr$ reduces to

$$P = -4\pi(e^{-at}-e^{-bt})/(a^2t-b^2t) \qquad .....(A.2)$$

Also $\int e^{-ar}e^{-b|\vec{r}-\vec{t}|}|r-t|^{-1}d\vec{r} = -dP/da$

$$= -4\pi(e^{-at}+2a(e^{-at}-e^{-bt})/(a^2t-b^2t))/(a^2-b^2) \qquad .....(A.3)$$

$$\int e^{-ar}e^{-b|\vec{r}-\vec{t}|}r^{-1}d\vec{r} = -dP/db$$

$$= 4\pi(e^{-bt}+2b(e^{-at}-e^{-bt})/(a^2t-b^2t))/(a^2-b^2) \qquad .....(A.4)$$

$$\int e^{-ar}e^{-b|\vec{r}-\vec{t}|}d\vec{r} = d^2P/dadb$$

$$=8\pi(be^{-at}+ae^{-bt}+4ab(e^{-at}-e^{-bt})/(a^2t-b^2t))/(a^2-b^2)^2 \qquad .....(A.5)$$

Various properties of the spherical harmonics, Y_ℓ^m, and Clebsch-Gordon coefficients, C's, are given by Rose(1957). For example, the orthonormalization formula for spherical harmonics is

$$\int \overset{*}{Y}{}_{\ell_1}^{m_1}(\Omega_r)Y_{\ell_2}^{m_2}(\Omega_r)d\Omega_r = \delta_{\ell_1\ell_2}\delta_{m_1m_2} \qquad .....(A.6)$$

where the δ's are kronecker delta functions, and Ω_r is the spherical coordinate labelled by the appropriate subscript to indicate the particular coordinate involved. Also there is the Addition Theorem for spherical harmonics

$$P_\ell(\cos\theta_{12}) = 4\pi\sum_m \overset{*}{Y}{}_\ell^m(\Omega_1)Y_\ell^m(\Omega_2)/(2\ell+1) \qquad .....(A.7)$$

where P_ℓ is the Legendre polynomial, θ_{12} is the angle between the coordinates labelled by 1 and 2, and unless otherwise indicated it shall be understood that the summation $\sum_m$ is from $m=-\ell$ to $m=+\ell$. Another useful property is

$$\int Y^{*m_3}_{\ell_3}(\Omega) Y^{m_2}_{\ell_2}(\Omega) Y^{m_1}_{\ell_1}(\Omega) d\Omega = ((2\ell_1+1)(2\ell_2+1))^{\frac{1}{2}} \times C(\ell_1 \ell_2 \ell_3; m_1 m_2 m_3) C(\ell_1 \ell_2 \ell_3; 000)/(4\pi(2\ell_3+1))^{\frac{1}{2}} \quad \text{.....(A.8)}$$

where the C's are Clebsch-Gordon coefficients.

Using a similar notation to that of Fraser (1961), define $G_\ell(\alpha,\beta,\sigma,r_p,m,n) \equiv G_\ell(\alpha,\beta,\sigma,m,n)$ where the r_p dependence will be suppressed, by

$$G_\ell(\alpha,\beta,\sigma,m,n) = \int (\sigma r_p/2)\, e^{-\alpha|\vec{\sigma}-\vec{r}_p| - \beta|2\vec{\sigma}-\vec{r}_p|} |2\vec{\sigma}-\vec{r}_p|^m \times |\vec{\sigma}-\vec{r}_p|^n P_\ell(\mu) d\mu \quad \text{.....(A.9)}$$

where $\mu = \vec{\sigma}\cdot\vec{r}_p/\sigma r_p$ and $P_\ell(\mu)$ is the Legendre polynomial.

Suppose

$$I_1 = \int e^{-\alpha_1|\vec{\sigma}_1-\vec{r}_p| - \beta_1|2\vec{\sigma}_1-\vec{r}_p|} |2\vec{\sigma}_1-\vec{r}_p|^{m_1} |\vec{\sigma}_1-\vec{r}_p|^{n_1} d\vec{\sigma}_1$$

This integrand may be expanded in terms of Legendre polynomials. Using equations (A.7) and (A.9), I_1 becomes

$$I_1 = \int (4\pi/\sigma_1 r_p) \sum_{\ell,m} G_\ell(\alpha_1,\beta_1,\sigma_1,m_1,n_1) Y^m_\ell(\Omega_{r_p}) Y^{*m}_\ell(\Omega_{\sigma_1})$$

$$x(4\pi)^{\frac{1}{2}}\, Y_o^o(\Omega_{\sigma_1})\sigma_1^2 d\Omega_{\sigma_1} d\sigma_1$$

Unless otherwise indicated the summation for ℓ is from $\ell=0$ to $\ell=\infty$. Note that $(4\pi)^{\frac{1}{2}}\, Y_o^o(\Omega_{\sigma_1})=1$ has been inserted. Integration over Ω_{σ_1} gives $\delta_{\ell o}\delta_{mo}$ using equation (A.6).

$$I_1 = \int((4\pi)^{\frac{3}{2}}\, \sigma_1/r_p) G_o(\alpha_1,\beta_1,\sigma_1,m_1,n_1) \overset{*}{Y}{}_o^o(\Omega_{r_p}) d\sigma_1 \qquad \text{.....(A.10)}$$

Similarly, the integral

$$I_2 = \int e^{-\alpha 2|\vec{\sigma}_2-\vec{r}_p|} -\beta 2|2\vec{\sigma}_2-\vec{r}_p| \,|2\vec{\sigma}_2-\vec{r}_p|^{m_2} |\vec{\sigma}_2-\vec{r}_p|^{n_2} d\vec{\sigma}_2$$

becomes

$$I_2 = \int((4\pi)^{\frac{3}{2}}\, \sigma_2/r_p) G_o(\alpha_2,\beta_2,\sigma_2,m_2,n_2) Y_o^o(\Omega_{r_p}) d\sigma_2 \qquad \text{.....(A.11)}$$

Hence the integral

$$I = \int I_1 I_2 d\vec{r}_p$$

becomes (combining equations (A.10) and (A.11))

$$I = \int((4\pi)^3 \sigma_1 /r_p) G_o(\alpha_1,\beta_1,\sigma_1,m_1,n_1) Y_o^o(\Omega_{r_p}) \sigma_2$$

$$x G_o(\alpha_2,\beta_2,\sigma_2,m_2,n_2) Y_o^o(\Omega_{r_p}) r_p d\Omega_{r_p} d\sigma_1 d\sigma_2 dr_p$$

Integration over Ω_{r_p} gives

$$I = (4\pi)^3 \int \sigma_1\sigma_2 G_o(\alpha_1,\beta_1,\sigma_1,m_1,n_1) G_o(\alpha_2,\beta_2,\sigma_2,m_2,n_2)$$

$$x d\sigma_1 d\sigma_2 dr_p \qquad \text{.....(A.12)}$$

Now (using equation (A.7))

$$\vec{\sigma}\cdot\vec{r}_p = \sigma r_p \cos\theta = \sigma r_p P_1(\cos\theta)$$

$$= \sigma r_p \sum_{m=-1}^{1} (4\pi/3) \overset{*}{Y}{}_1^m(\Omega_{\sigma_1}) Y_1^m(\Omega_{r_p}) \qquad \text{.....(A.13)}$$

Suppose

$$I_3 = \int e^{-\alpha_1 |\vec{\sigma}_1 - \vec{r}_p|} - \beta_1 |2\vec{\sigma}_i - \vec{r}_p| \, |2\vec{\sigma}_1 - \vec{r}_p|^{m_1} |\vec{\sigma}_1 - \vec{r}_p|^{n_1} \vec{\sigma}_1 \cdot \vec{r}_p d\vec{\sigma}_1$$

From equations (A.6) and (A.13), proceeding as before,

$$I_3 = \int \sigma_1 r_p (4\pi/3) \sum_{m_o=-1}^{1} \overset{*}{Y}{}_1^{m_o}(\Omega_{\sigma_1}) Y_1^{m_o}(\Omega_{r_p}) (4\pi/\sigma_1 r_p)$$

$$\times \sum_{\ell_3, m_3} Y_{\ell_3}^{m_3}(\Omega_{\sigma_1}) \overset{*}{Y}{}_{\ell_3}^{m_3}(\Omega_{r_p}) G_{\ell_3}(\alpha_1, \beta_1, \sigma_1, m_1, n_1) \sigma_1^2 d\Omega_{\sigma_1} d\sigma_1$$

Integration over Ω_{σ_1} gives $\delta_{\ell_3 1} \delta_{m_3 m_o}$ using equation (A.6)

Hence

$$I_3 = \int ((4\pi)^2/3) \sum_{m_o=-1}^{1} Y_1^{m_o}(\Omega_{r_p}) \overset{*}{Y}{}_1^{m_o}(\Omega_{r_p}) G_1(\alpha_1, \beta_1, \sigma_1, m_1, n_1)$$

$$\times \sigma_1^2 d\sigma_1 \qquad \text{.....(A.14)}$$

Thus the integral

$$I = \int I_3 I_2 d\vec{r}_p$$

becomes (combining equations (A.11) and (A.14))

$$I = \int \sigma_1^2 ((4\pi)^{\frac{7}{2}}/3 r_p) \sigma_2 G_1(\alpha_1, \beta_1, \sigma_1, m_1, n_1) G_o(\alpha_2, \beta_2, \sigma_2, m_2,$$

$$n_2) \sum_{m_o=-1}^{1} \overset{*}{Y}{}_1^{m_o}(\Omega_{r_p}) Y_1^{m_o}(\Omega_{r_p}) Y_o^o(\Omega_{r_p}) r_p^2 d\Omega_{r_p} d\sigma_1 d\sigma_2 dr_p$$

Using equation (A.8), the integral reduces to

$$I = \int \sigma_1^2 \sigma_2 r_p (4\pi)^3 G_1(\alpha_1,\beta_1,\sigma_1,m_1,n_1) G_o(\alpha_2,\beta_2,\sigma_2,m_2,n_2)$$

$$x d\sigma_1 d\sigma_2 dr_p \qquad \text{.....(A.15)}$$

Similarly, $|\vec{\sigma}_1 - \vec{\sigma}_2|^{-1}$ may be expanded in terms of Legendre polynomials. Using equation (A.7) on such an expansion gives

$$|\vec{\sigma}_1 - \vec{\sigma}_2|^{-1} = \sum_{\ell,m} (4\pi/(2\ell+1)) \gamma_\ell(\sigma_1,\sigma_2) \overset{*}{Y}{}_\ell^m(\Omega_{\sigma_1}) Y_\ell^m(\Omega_{\sigma_2})$$

where

$$\gamma_\ell(\sigma_1,\sigma_2) = \sigma_1^\ell / \sigma_2^{\ell+1} \quad \text{if} \quad \sigma_1 \leq \sigma_2$$

and

$$\gamma_\ell(\sigma_1,\sigma_2) = \sigma_2^\ell / \sigma_1^{\ell+1} \quad \text{if} \quad \sigma_1 \geq \sigma_2 \qquad \text{.....(A.16)}$$

Suppose

$$I = \int e^{-\alpha_1 |\vec{\sigma}_1 - \vec{r}_p|} |\vec{\sigma}_1 - \vec{r}_p|^{-\beta_1} |2\vec{\sigma}_1 - \vec{r}_p|^{m_1} |\vec{\sigma}_1 - \vec{r}_p|^{n_1} |\vec{\sigma}_1 - \vec{\sigma}_2|^{-1}$$

$$x e^{-\alpha_2 |\vec{\sigma}_2 - \vec{r}_p|} |\vec{\sigma}_2 - \vec{r}_p|^{-\beta_2} |2\vec{\sigma}_2 - \vec{r}_p|^{m_2} |\vec{\sigma}_2 - \vec{r}_p|^{n_2} d\vec{\sigma}_1 d\vec{\sigma}_2 d\vec{r}_p$$

Proceeding as before, using equation (A.16), I becomes

$$I = \int (4\pi/\sigma_1 r_p) \sum_{\ell_4,m_4} G_{\ell_4}(\alpha_1,\beta_1,\sigma_1,m_1,n_1) Y_{\ell_4}^{m_4}(\Omega_{\sigma_1})$$

$$x \overset{*}{Y}{}_{\ell_4}^{m_4}(\Omega_{r_p}) \sum_{\ell_5,m_5} (4\pi/\sigma_2 r_p) G_{\ell_5}(\alpha_2,\beta_2,\sigma_2,m_2,n_2) \overset{*}{Y}{}_{\ell_5}^{m}(\Omega_{\sigma_2})$$

$$x Y_{\ell_5}^{m_5}(\Omega_{r_p}) \sum_{\ell_3,m_3} (4\pi/(2\ell_3+1)) \gamma_{\ell_3}(\sigma_1,\sigma_2) \overset{*}{Y}{}_{\ell_3}^{m_3}(\Omega_{\sigma_1}) Y_{\ell_3}^{m_3}(\Omega_{\sigma_2})$$

$$x \sigma_1^2 d\Omega_{\sigma_1} d\sigma_1 \sigma_2^2 d\Omega_{\sigma_2} d\sigma_2 r_p^2 d\Omega_{r_p} dr_p$$

Using equation (A.6), I reduces to

$$I = (4\pi)^3 \int \sigma_1 \sigma_2 \sum_{\ell=0}^{\infty} G_\ell(\alpha_1,\beta_1,\sigma_1,m_1,n_1) G_\ell(\alpha_2,\beta_2,\sigma_2,m_2,n_2)$$

$$x\gamma_\ell(\sigma_1,\sigma_2) d\sigma_1 d\sigma_2 dr_p \qquad \text{.....(A.17)}$$

In an analogous fashion, various integrals may be expressed in terms of J where

$$J_\ell(\alpha,\beta,r,m,n) = (rr_p/2)\int e^{-\alpha|\vec{r}-\vec{r}_p| - \beta r} |\vec{r}-\vec{r}_p|^n r^m P_\ell(\mu) d\mu$$

with $\mu = \vec{r}\cdot\vec{r}_p/rr_p$ .....(A.18)

For example,

$$\int e^{-\alpha_1|\vec{r}_1-\vec{r}_p| - \beta_1 r_1} r_1^{m_1} |\vec{r}_1-\vec{r}_p|^{n_1} e^{-\alpha_2|\vec{r}_2-\vec{r}_p| - \beta_2 r_2} r_2^{m_2}$$

$$x|\vec{r}_2-\vec{r}_p|^{n_2} d\vec{r}_1 d\vec{r}_2 d\vec{r}_p$$

$$= (4\pi)^3 \int J_o(\alpha_1,\beta_1,r_1,m_1,n_1) J_o(\alpha_2,\beta_2,r_2,m_2,n_2) r_1 r_2$$

$$x dr_1 dr_2 dr_p \qquad \text{.....(A.19)}$$

$$\int e^{-\alpha_1|\vec{r}_1-\vec{r}_p| - \beta_1 r_1} r_1^{m_1} |\vec{r}_1-\vec{r}_p|^{n_1} e^{-\alpha_2|\vec{r}_2-\vec{r}_p| - \beta_2 r_2} r_2^{m_2}$$

$$x|r_2-r_p|^{n_2} \vec{r}_1\cdot\vec{r}_p d\vec{r}_1 d\vec{r}_2 d\vec{r}_p$$

$$= (4\pi)^3 \int r_p J_1(\alpha_1,\beta_1,r_1,m_1,n_1) J_o(\alpha_2,\beta_2,r_2,m_2,n_2) r_1^2 r_2$$

$$x dr_1 dr_2 dr_p \qquad \text{.....(A.20)}$$

$$\int e^{-\alpha_1|\vec{r}_1-\vec{r}_p|-\beta_1 r_1}\, r_1^{m_1}|\vec{r}_1-\vec{r}_p|^{n_1} e^{-\alpha_2|\vec{r}_2-\vec{r}_p|-\beta_2 r_2}\, r_2^{m_2}$$

$$x|\vec{r}_2-\vec{r}_p|^{n_2}|\vec{r}_1-\vec{r}_2|^{-1} d\vec{r}_1 d\vec{r}_2 d\vec{r}_p$$

$$=(4\pi)^3 \int \sum_{\ell=0}^{\infty} r_1 r_2 J_\ell(\alpha_1,\beta_1,r_1,m_1,n_1)\gamma_\ell(r_1,r_2)$$

$$xJ_\ell(\alpha_2,\beta_2,r_2,m_2,n_2)dr_1 dr_2 dr_p$$

.....(A.21)

APPENDIX B

EVALUATION OF MATRIX ELEMENTS

B.1 o-Ps-He System

(a) Scattering Length

The various reductions of integration and use of the functions G_ℓ and J_ℓ outlined in Appendix A are exploited in doing these calculations. As these calculations are quite straightforward, only a brief summary is given.

$$A = (v/\sigma, v/\sigma)$$

$$= \int \phi_1 \psi_{23} (v_1/\sigma_1)(H-E)\phi_1 \psi_{23} (v_1/\sigma_1) d\tau$$

$$- \int \phi_1 \psi_{23} (v_1/\sigma_1)(H-E)\phi_2 \psi_{13} (v_2/\sigma_2) d\tau \qquad \text{.....(B.1)}$$

It may be shown that the direct term (that is, the first term) is identically zero and that the exchange term (that is, the second term) reduces to

$$A)_{\text{exchange}} = -\int \phi_1 \phi_2 \psi_{23} (v_1/\sigma_1)(v_2/\sigma_2) N_1 \sum_{i=1}^{M} u_i \, e^{-x_i r_1}$$

$$\times e^{-y_i r_3} \left(\Delta((2x_i-4)/r_1 + (2y_i-4)/r_3 + 2/|\vec{r}_1-\vec{r}_3| - x_i^2-y_i^2\right.$$

$$\left. -E_{He}\right) - 4/r_2 + 4/r_p - 2/|\vec{r}_1-\vec{r}_p| - 2/|\vec{r}_3-\vec{r}_p| + 2/|\vec{r}_1-\vec{r}_2|$$

$$+ 2/|\vec{r}_2-\vec{r}_3|) d\tau \qquad \text{.....(B.2)}$$

This integral may be written as

$$A)_{\text{exchange}} = 512N_1^2\pi^3 \int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d v_1 v_2 \left(\frac{8}{y_{id}}\right)^3 (G_o(1,x_i,\sigma_1,0,0)$$

$$x((-2/r_p-(y_{id}+2/r_p)e^{-y_{id}r_p})G_o(1,x_d,\sigma_2,0,0)$$

$$+2G_o(1,x_d,\sigma_2,-1,0)+y_{id}G_o(1,x_d+y_{id},\sigma_2,0,0)$$

$$+2G_o(1,x_d+y_{id},\sigma_2,-1,0))+G_o(1,x_d,\sigma_2,0,0)$$

$$x(G_o(1,x_i,\sigma_1,0,-1)+\Delta((x_i^2+y_i^2+E_{He}+(2-y_i)y_{id})$$

$$xG_o(1,x_i,\sigma_1,0,0)+(2-2x_i)G_o(1,x_i,\sigma_1,-1,0)$$

$$+y_{id}G_o(1,x_i+y_{id},\sigma_1,0,0)+2G_o(1,x_i+y_{id},\sigma_1,-1,0)))$$

$$-\sum_{\ell=0}^{\infty} G_\ell(1,x_i,\sigma_1,0,0)G_\ell(1,x_d,\sigma_2,0,0)\gamma_\ell(\sigma_1,\sigma_2))d\sigma_1 d\sigma_2 dr_p$$

.....(B.3)

where $y_{id}=y_i+y_d$. Note that $\Delta=0$ corresponds to the "Pseudo-exact" case and $\Delta=1$ the "Inexact" case described in Chapter 3, Sections 3 and 4.

$$B = (v/\sigma,w/\sigma)+(w/\sigma,v/\sigma) \qquad .....(B.4)$$

Here it may be shown that the direct term of B reduces to

$$B_{\text{direct}} = -\frac{1}{2}\int (v_1/\sigma_1^2)(d^2w_1/d\sigma_1^2)4\pi\sigma_1^2 d\sigma_1$$

$$=-2\pi\int(-\sigma_1)(-\delta^2 e^{-\delta\sigma_1})d\sigma_1 \quad =-2\pi \qquad .....(B.5)$$

The exchange term is the same as that given for A (that is, equation (B.3)) replacing the product v_1v_2 by $(v_1w_2+v_2w_1)$ with the addition of the term

$$256N_1^2\pi^3\int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d \left(\frac{8}{y_{id}}\right)^3 v_1(-\delta^2 e^{-\delta\sigma_1})G_o(1,x_i,\sigma_1,0,0)$$

$$xG_o(1,x_d,\sigma_2,0,0)d\sigma_1 d\sigma_2 dr_p \qquad \text{.....(B.6)}$$

$$C = (w/\sigma, w/\sigma) \qquad \text{.....(B.7)}$$

In this case the direct term reduces to

$$C_{direct} = -(1/2)\int (w_1/\sigma_1^2)\,(d^2w_1/d\sigma_1^2)4\pi\sigma_1^2 d\sigma_1$$

$$=-2\pi\int (1-e^{-\delta\sigma_1})\,(-\delta^2 e^{-\delta\sigma_1})d\sigma_1 = \pi\delta \qquad \text{.....(B.8)}$$

The exchange term is the same as that given for A (equation (B.3)) replacing the product v_1v_2 by w_1w_2 with the addition of the term

$$256N_1^2\pi^3\int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d \left(\frac{8}{y_{id}}\right)^3 w_1(-\delta^2 e^{-\delta\sigma_1})G_o(1,x_i,\sigma_1,0,0)$$

$$xG_o(1,x_d,\sigma_2,0,0)d\sigma_1 d\sigma_2 dr_p \qquad \text{.....(B.9)}$$

$$D_k = (v/\sigma, f_k/\sigma) + (f_k/\sigma, v/\sigma) \qquad \text{.....(B.10)}$$

In this case, it may be shown that the direct term is identically zero. Here $D_k)_{exchange}$ is the same as that given for A (equation (B.3)) replacing the product v_1v_2 by

$(v_1 f_k^{(2)} + f_k^{(1)} v_2)$ with the addition of the term

$$256N_1^2\pi^3 \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d \frac{8}{(\overline{yid})^3} v_1 (k(k-1)\sigma_2^{k-2} - 2k\delta\sigma_2^{k-1} + \delta^2\sigma_2^k)$$

$$xe^{-\delta\sigma_2} G_o(1,x_i,\sigma_1,0,0) G_o(1,x_d,\sigma_2,0,0) d\sigma_1 d\sigma_2 dr_p$$

.....(B.11)

$$E_k = (w/\sigma, f_k/\sigma) + (f_k/\sigma, w/\sigma) \qquad .....(B.12)$$

In this case, the direct term reduces to

$$E_k)_{direct} = -(1/2)\ (f_k^{(1)}/\sigma_1^2)(d^2 w_1/d\sigma_1^2) 4\pi\sigma_1^2 d\sigma_1$$

$$-(1/2)\ (w_1/\sigma_1^2)(d^2 f_k^{(1)}/d\sigma_1^2) 4\pi\sigma_1^2 d\sigma_1$$

$$= \frac{\pi k!}{(2\delta)}\ k-1 \qquad .....(B.13)$$

The exchange term is the same as that given for A (equation (B.3)) replacing the product $v_1 v_2$ by $(w_1 f_k^{(2)} + f_k^{(1)}\ w_2)$ with the addition of the term

$$256N_1^2\pi^3 \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d \frac{8}{(\overline{yid})^3} (w_1 (k(k-1)/\sigma_2^2 - 2k\sigma/\sigma_2 + \delta^2)\sigma_2^k e^{-\delta\sigma_2}$$

$$+ f_k^{(1)}\ (-\delta^2 e^{-\delta\sigma_2})) G_o(1,x_i,\sigma_1,0,0) G_o(1,x_d,\sigma_2,0,0) d\sigma_1 d\sigma_2$$

$$xdr_p \qquad .....(B14)$$

$$F_{jk} = (f_j/\sigma, f_k/\sigma) = F_{kj} \qquad \text{.....(B.15)}$$

In this case, the direct term reduces to

$$F_{jk)_{\text{direct}}} = -(1/2)\int (f_j^{(1)}/\sigma_1^2)(d^2 f_k^{(1)}/d\sigma_1^2)4\pi\sigma_1^2 d\sigma_1$$

$$= -2\pi(-jk+(j+k)(j+k-1)/4)(j+k-1)!)/(2\delta)^{j+k-2}$$

$$\text{.....(B.16)}$$

$F_{jk)_{\text{exchange}}}$ is the same as that given for A (equation (B.3))replacing the product $v_1 v_2$ by $f_j^{(1)} f_k^{(2)}$ with the addition of the term

$$256 N_f^2 \pi^3 \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d \frac{8}{(yid)^3} f_j^{(1)}(k(k-1)/\sigma_2^2 - 2k\delta/\sigma_2 + \delta^2)$$

$$x\sigma_2^k \, e^{-\delta\sigma_2} G_o(1, x_i, \sigma_1, 0, 0) G_o(1, x_d, \sigma_2, 0, 0) d\sigma_1 d\sigma_2 dr_p$$

$$\text{.....(B.17)}$$

Now

$$\nabla_1^2 \phi_1 X_k^{(1)} = \nabla_1 \cdot \phi_1 X_k^{(1)}((q_k/r_1 - \gamma)\vec{r}_1/r_1 + (m_k/|\vec{r}_1 - \vec{r}_p|$$

$$-1/2+\beta)(\vec{r}_1 - \vec{r}_p)/|\vec{r}_1 - \vec{r}_p|)$$

$$= \phi_1 X_k^{(1)}(q_k(q_k+1)/r_1^2 - 2\gamma(q_k+1)/r_1 + \gamma^2$$

$$+(q_k/r_1 - \gamma)(2m_k/|\vec{r}_1 - \vec{r}_p| - 1 - 2\beta)\vec{r}_1 \cdot (\vec{r}_1 - \vec{r}_p)/r_1 |\vec{r}_1 - \vec{r}_p|$$

$$+m_k(m_k+1)/|\vec{r}_1 - \vec{r}_p|^2 - (1-2\beta)(m_k+1)/|\vec{r}_1 - \vec{r}_p| + (\beta - 1/2)^2)$$

$$\nabla_p^2\phi_1\chi_k^{(1)} = \nabla_p\cdot\phi_1\chi_k^{(1)}((h_k/r_p-\eta)\vec{r}_p/r_p+(-m_k/|\vec{r}_1-\vec{r}_p| +1/2-\beta)(\vec{r}_1-\vec{r}_p)/|\vec{r}_1-\vec{r}_p|)$$

$$= \phi_1\chi_k^{(1)}(h_k(h_k+1)/r_p^2-2\eta(h_k+1)/r_p+\eta^2$$

$$-(h_k/r_p-\eta)(2m_k/|\vec{r}_1-\vec{r}_p|-1+2\beta)\vec{r}_p\cdot(\vec{r}_1-\vec{r}_p)/(r_p|\vec{r}_1-\vec{r}_p|)$$

$$+m_k(m_k+1)/|\vec{r}_1-\vec{r}_p|^2-(1-2\beta)(m_k+1)/|\vec{r}_1-\vec{r}_p|+(\beta-1/2)^2)$$

.....(B.18)

For convenience, define

$$Q(\alpha_1,\beta_1,\sigma,q_1,m_1,\beta,\gamma,\eta,h,q,m)=q(q+1)G_o(\alpha_1,\beta_1,\sigma,q_1-2,m_1)$$

$$-2\gamma(q+1)G_o(\alpha_1,\beta_1,\sigma,q_1-1,m_1)+0.5m(m+1)G_o(\alpha_1,\beta_1,\sigma,q_1,m_1-2)$$

$$+(-m+2\beta(m+1))G_o(\alpha_1,\beta_1,\sigma,q_1,m_1-1)$$

$$+qm((2\sigma^2+r_p^2)G_o(\alpha_1,\beta_1,\sigma,q_1-2,m_1-2)$$

$$-3\sigma r_p G_1(\alpha_1,\beta_1,\sigma,q_1-2,m_1-2))$$

$$-(1-2\beta)q((2\sigma^2+r_p^2)G_o(\alpha_1,\beta_1,\sigma,q_1-2,m_1-1)$$

$$-3\sigma r_p G_1(\alpha_1,\beta_1,\sigma,q_1-2,m_1-1))$$

$$-m\gamma((2\sigma^2+r_p^2)G_o(\alpha_1,\beta_1,\sigma,q_1-1,m_1-2)$$

$$-3\sigma r_p G_1(\alpha_1,\beta_1,\sigma,q_1-1,m_1-2))$$

$$+(1-2\beta)\gamma((2\sigma^2+r_p^2)G_o(\alpha_1,\beta_1,\sigma,q_1-1,m_1-1)$$

$$-3\sigma r_p G_1(\alpha_1,\beta_1,\sigma,q_1-1,m_1-1))$$

$$-(h/r_p-\eta)m(\sigma G_1(\alpha_1,\beta_1,\sigma,q_1,m_1-2)-r_p G_o(\alpha_1,\beta_1,\sigma,q_1,m_1-2))$$

$$+(h/r_p-\eta)(1-2\beta)(\sigma G_1(\alpha_1,\beta_1,\sigma,q_1,m_1-1)$$

$$-r_p G_o(\alpha_1,\beta_1,\sigma,q_1,m_1-1))+(\gamma^2+2\beta^2-2\beta+h(h+1)/r_p$$

$$-2\eta(h+1)/r_p+\eta^2)G_o(\alpha_1,\beta_1,\sigma,q_1,m_1) \qquad .....(B.19)$$

and

$$L(\alpha_1,\beta_1,r,q_1,m_1,\beta,\gamma,\eta,h,q,m)=(q(q+1)/r^2-2\gamma(q+1)/r+\gamma^2+2\beta^2$$

$$-2\beta+h(h+1)/r_p^2-2\eta(h+1)/r_p+\eta^2)J_o(\alpha_1,\beta_1,r,q_1,m_1)$$

$$+2m(m+1)J_o(\alpha_1,\beta_1,r,q_1,m_1-2)$$

$$+2(-m+2\beta(m+1))J_o(\alpha_1,\beta_1,r,q_1,m_1-1)$$

$$+(q/r-\gamma)m(rJ_o(\alpha_1,\beta_1,r,q_1,m_1-2)-r_p J_1(\alpha_1,\beta_1,r,q_1,m_1-2))$$

$$-(q/r-\gamma)(1-2\beta)(rJ_o(\alpha_1,\beta_1,r,q_1,m_1-1)-r_p J_1(\alpha_1,\beta_1,r,q_1,m_1-1))$$

$$-(h/r_p-\eta)m(rJ_1(\alpha_1,\beta_1,r,q_1,m_1-2)-r_p J_o(\alpha_1,\beta_1,r,q_1,m_1-2))$$

$$+(h/r_p-\eta)(1-2\beta)(rJ_1(\alpha_1,\beta_1,r,q_1,m_1-1)$$

$$-r_p J_o(\alpha_1,\beta_1,r,q_1,m_1-1)) \qquad .....(B.20)$$

Now

$$R_k=(v/\sigma,\chi_k)+(\chi_k,v/\sigma) \qquad .....(B.21)$$

It may be shown that the direct term reduces to

$$R_k)_{direct}=-2\int\phi_1^2\psi_{23}(v/\sigma_1)\chi_k^{(1)}N\sum_{i=1}^{M}u_i e^{-y_i r_1}(q_k(q_k+1)/r_1^2$$

$$+(4-2\gamma(q_k+1))/r_1+\gamma^2+h_k(h_k+1)/r_p^2-(4+2\eta(h_k+1))/r_p+\eta^2$$

$$+2m_k(m_k+1)/|\vec{r}_1-\vec{r}_p|^2+2(-m_k+2\beta(m_k+1))/|\vec{r}_1-\vec{r}_p|+2\beta^2-2\beta$$

$$+(q_k/r_1-\gamma)(2m_k/|\vec{r}_1-\vec{r}_p|-1+2\beta)\vec{r}_1\cdot(\vec{r}_1-\vec{r}_p)/r_1|\vec{r}_1-\vec{r}_p|$$

$$-(h_k/r_p-\eta)(2m_k/|\vec{r}_1-\vec{r}_p|-1+2\beta)\vec{r}_p\cdot(\vec{r}_1-\vec{r}_p)/r_p|\vec{r}_1-\vec{r}_p|$$

$$+2/|\vec{r}_2-\vec{r}_p|+2/|\vec{r}_3-\vec{r}_p|-2/|\vec{r}_1-\vec{r}_2|-2/|\vec{r}_1-\vec{r}_3|)d\tau$$

$$= -32N_1^2\pi^3\int\sum_{\substack{i=1\\d=1}}^{M}u_iu_d\frac{8}{(y_{id})^3}\frac{8}{(x_{id})^3}r_p^{h_k+1}\,e^{-\eta r_p}\,v_1$$

$$x\ (Q(2-2\beta,\gamma,\sigma_1,q_k,m_k,\beta,\gamma,\eta,h_k,q_k,m_k)$$

$$+y_{id}G_o(2-2\beta,\gamma+y_{id},\sigma_1,q_k,m_k)+x_{id}G_o(2-2\beta,\gamma+x_{id},\sigma_1,q_k,m_k)$$

$$+2G_o(2-2\beta,\gamma+y_{id},\sigma_1,q_k-1,m_k)+2G_o(2-2\beta,\gamma+x_{id},\sigma_1,q_k-1,m_k)$$

$$+(-(y_{id}+2/r_p)e^{-y_{id}r_p}-(x_{id}+2/r_p)e^{-x_{id}r_p})$$

$$x\ G_o(2-2\beta,\gamma,\sigma_1,q_k,m_k))d\sigma_1 dr_p \qquad .....(B.22)$$

where $x_{id}=x_i+x_d$.

By operating the Hamiltonian to the left instead of to the right, it may be shown that $R_k)_{direct}$ becomes

$$R_k)_{direct} = -2\int\phi_1^2\psi_{23}v_1/\sigma_1\chi_k^{(1)}N_1\sum_{i=1}^{M}u_ie^{-y_ir_3}(4/r_1-4/r_p$$

$$+2/|\vec{r}_2-\vec{r}_p|+2/|\vec{r}_3-\vec{r}_p|-2/|\vec{r}_1-\vec{r}_2|-2/|\vec{r}_1-\vec{r}_3|)d\tau$$

$$= -32N_1^2\pi^3\int\sum_{\substack{i=1\\d=1}}^{M}u_iu_d\frac{8}{(y_{id})^3}\frac{8}{(x_{id})^3}r_p^{h_k+1}\,e^{-\eta r_p}\,v_1$$

$$x\ (y_{id}G_o(2-2\beta,\gamma+y_{id},\sigma_1,q_k,m_k)+x_{id}G_o(2-2\beta,\gamma+x_{id},\sigma_1,q_k,m_k)$$

$$+2G_o(2-2\beta,\gamma+y_{id},\sigma_1,q_k-1,m_k)+2G_o(2-2\beta,\gamma+x_{id},\sigma_1,q_k-1,m_k)$$

$$+(-(y_{id}+2/r_p)e^{-y_{id}r_p}-(x_{id}+2/r_p)e^{-x_{id}r_p)}$$

$$x\ G_o(2-2\beta,\gamma,\sigma_1,q_k,m_k)d\sigma_1 dr_p \qquad .....(B.23)$$

As this expression must give the same value of $R_k)_{direct}$ as given by equation (B.22) it provides a useful check on the consistency of the code used in the computer and also on the accuracy of the integration technique used.

Similarly, the exchange term reduces to

$$R_k)_{exchange}=\int\phi_1\psi_{23}(v_1/\sigma_1)\chi_k^{(2)}N_1^2\sum_{\substack{i=1\\d=1}}^{M}u_iu_d e^{-x_ir_1}e^{-x_dr_2}e^{-y_{id}r_3}$$

$$x(q_k(q_k+1)/r_2^2+(4-2\gamma(q_k+1))/r_2+\ h_k(h_k+1)/r_p^2+\gamma^2$$

$$-(4+2\eta(h_k+1))/r_p+\eta^2+2m_k(m_k+1)/|\vec{r}_2-\vec{r}_p|^2-2/|\vec{r}_1-\vec{r}_2|$$

$$+2(-m_k+2\beta(m_k+1))/|\vec{r}_2-\vec{r}_p|+2\beta^2-2\beta+2/|\vec{r}_1-\vec{r}_p|+2/|\vec{r}_3-\vec{r}_p|$$

$$+(q_k/r_2-\gamma)(2m_k/|\vec{r}_2-\vec{r}_p|-1+2\beta)\vec{r}_2\cdot(\vec{r}_2-\vec{r}_p)/r_2|\vec{r}_2-\vec{r}_p|$$

$$-(h_k/r_p-\eta)(2m_k/|\vec{r}_2-\vec{r}_p|-1+2\beta)\vec{r}_p\cdot(\vec{r}_2-\vec{r}_p)/r_p|\vec{r}_2-\vec{r}_p|$$

$$+\Delta((4-2x_i)/r_1+(4-2y_i)/r_3+x_i^2+y_i^2+E_{He}-2/|\vec{r}_1-\vec{r}_3|))d\tau$$

$$+\int\phi_1\phi_2\psi_{23}(v_2/\sigma_2)\chi_k^{(1)}N_1^2\sum_{i=1}^{M}u_i e^{-x_ir_1}e^{-y_ir_3}(\Delta((4-2x_i)/r_1$$

$$+(4-2y_i)/r_3-2/|\vec{r}_1-\vec{r}|_3+x_i^2+y_i^2+E_{He})+4/r_2-4/r_p+2/|\vec{r}_1-\vec{r}_p|$$

$$+2/|\vec{r}_3-\vec{r}_p|-2/|\vec{r}_1-\vec{r}_2|\ -2/|\vec{r}_2-\vec{r}_3|)d\tau$$

$$= 128N_1^2\pi^3\int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d v_1 r_2 \left(\frac{8}{y_{id}}\right)^3 r_p^{h_k} e^{-\eta r_p} (G_o(1,x_i,\sigma_1,0,0)$$

$$x(L(0.5-\beta,\gamma+x_d,r_2,q_k,m_k,\beta,\gamma,\eta,h_k,q_k,m_k)+(2/r_2-2/r_p+(y_{id}$$

$$+2/r_2)e^{-y_{id}r_2}-(y_{id}+2/r_p)e^{-y_{id}r_p})J_o(0.5-\beta,\gamma+x_d,r_2,q_k,m_k)$$

$$+J_o(0.5-\beta,\gamma+x_d,r_2,q_k,m_k)(G_o(1,x_i,\sigma_1,0,-1)$$

$$+ ((2-2x_i)G_o(1,x_i,\sigma_1,-1,0)+y_{id}G_o(1,x_i+y_{id},\sigma_1,0,0)$$

$$+2G_o(1,x_i+y_{id},\sigma_1,-1,0)+(x_i^2+y_i^2+E_{He}+0.5y_{id}(4-2y_i))\Delta)$$

$$x\ G_o(1,x_i,\sigma_1,0,0))))d\sigma_1 dr_2 dr_p$$

$$-1024N_1^2\pi^3\int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d v_1 \sigma_2 \left(\frac{8}{y_{id}}\right)^3 r_p^{h_k} e^{-\eta r_p}\ G_\ell(1,x_i,\sigma_1,0,0)$$

$$x\ G_\ell(1-2\beta,\gamma+x_d,\sigma_2,q_k,m_k)\gamma_\ell(\sigma_1,\sigma_2)d\sigma_1 d\sigma_2 dr_p$$

$$+128N_1^2\pi^3\int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d v_2 r_1 \left(\frac{8}{y_{id}}\right)^3 r_p^{h_k} e^{-\eta r_p}($$

$$J_o(0.5-\beta,\gamma+x_i,r_1,q_k,m_k)((-2/r_p-(y_{id}+2/r_p)e^{-y_{id}r_p})$$

$$G_o(1,x_d,\sigma_2,0,0)+2G_o(1,x_d,\sigma_2,m-1,0)+y_{id}G_o(1,x_d+y_{id},\sigma_2,0,0)$$

$$+2G_o(1,x_d+y_{id},\sigma_2,-1,0))+G_o(1,x_d,\sigma_2,0,0)$$

$$(2J_o(0.5-\beta,\gamma+x_i,r_1,q_k,m_k-1)+\Delta((x_i^2+y_i^2+E_{He}+(2-y_i)y_{id}$$

$$+(2-2x_i)/r_1+(y_{id}+2/r_1)e^{-y_{id}r_1})J_o(0.5-\beta,\gamma+x_i,r_1,q_k,m_k)$$

$$x\ dr_1 d\sigma_2 dr_p \quad -1024N_1^2\pi^3 \int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d v_1 \sigma_2 (\frac{8}{y_{id}})^3 r_p^{hk}\ e^{-\eta r_p}$$

$$xG_{\ell}(1,x_i,\sigma_1,0,0)G_{\ell}(1-2\beta,\gamma+x_d,\sigma_2,q_k,m_k)\gamma_{\ell}(\sigma_1,\sigma_2)d\sigma_1 d\sigma_2 dr_p$$

.....(B.24)

$$H_k = (w/\sigma,\chi_k) + (\chi_k,w/\sigma) \qquad .....(B.25)$$

Here $H_k)_{direct}$ is the same as that given for $R_k)_{direct}$ (equation (B.22)) replacing v_1 with w_1. $H_k)_{exchange}$ is the same as that given for $R_k)_{exchange}$ in equation (B.24) replacing v_1 by w_1 in the first expression and v_2 by w_2 in the second expression with the addition of the term

$$128N_1^2\pi^3 \int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d (\frac{8}{y_{id}})^3 (-\delta^2 e^{-\delta\sigma_2}) G_o(1,x_d,\sigma_2,0,0)$$

$$x\ J_o(0.5-\beta,\gamma+x_i,r_1,q_k,m_k)dr_1 d\sigma_2 dr_p \qquad .....(B.26)$$

$$S_{jk} = (h_j/\sigma,\chi_k) + (\chi_k,h_j/\sigma) \qquad .....(B.27)$$

Here $S_{jk})_{direct}$ is the same as that given for $R_k)_{direct}$ (equation (B.22)) replacing v_1 by $h_j^{(1)}$. $S_{jk})_{exchange}$ is the same as that given for $R_k)_{exchange}$ in equation (B.24)

replacing v_1 by $h_j^{(1)}$ in the first integral and v_2 by $h_j^{(2)}$ in the second integral with the addition of the term

$$128N_1^2\pi^3 \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d \frac{8}{(y_{id})^3} (j(j-1)/\sigma_2 - 2j\delta/\sigma_2 + \delta^2)\sigma_2^j \, e^{-\delta\sigma_2}$$

$$x \; G_o(1, x_d, \sigma_2, 0, 0) J_o(0.5-\beta, \gamma+x_d, r_1, q_k, m_k) dr_1 d\sigma_2 dr_p$$

.....(B.28)

Here the direct term reduces to

$$K_{jk})_{direct} = -\int \phi_1^2 \psi_{23} \chi_j^{(1)} \chi_k^{(1)} N_1 \sum_{i=1}^{M} u_i e^{-x_i r_2} \, e^{-y_i r_2}$$

$$x(q_k(q_k+1)/r_1^2 + (4-2\gamma(q_k+1))/r_1 + \gamma^2 + h_k(h_k+1)/r_p^2$$

$$-(4+2\eta(h_k+1))/r_p + \eta^2 + 2m_k(m_k+1)/|\vec{r}_1-\vec{r}_p|^2 + 2\beta^2 - 2\beta + 2/|\vec{r}_2-\vec{r}_p|$$

$$+2(-m_k+2\beta(m_k+1))/|\vec{r}_1-\vec{r}_p| + 2/|\vec{r}_3-\vec{r}_p| - 2/|\vec{r}_1-\vec{r}_2| - 2/|\vec{r}_1-\vec{r}_3|$$

$$+(q_k/r_1-\gamma)(2m_k/|\vec{r}_1-\vec{r}_p| - 1 + 2\beta)\vec{r}_1 \cdot (\vec{r}_1-\vec{r}_p)/r_1|\vec{r}_1-\vec{r}_p|$$

$$-(h_k/r_p-\eta)(2m_k/|\vec{r}_1-\vec{r}_p| - 1 + 2\beta)\vec{r}_p \cdot (\vec{r}_1-\vec{r}_p)/r_p|\vec{r}_1-\vec{r}_p|$$

$$+\Delta((4-2x_i)/r_2 + (4-2y_i)/r_3 - 2/|r_2-r_3| + x_i^2 + y_i^2 + E_{He}))d\tau$$

$$= -2N_1^2\pi^3 \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d r_p^{h_j+h_k+1} \, e^{-2\eta r_p} \, \frac{8}{(y_{id})^3} \frac{8}{(x_{id})^3} r_1$$

$$x(L(1-2\beta, 2\gamma, r_1, q_j+q_k, m_j+m_k, \beta, \gamma, \eta, h_k, q_k, m_k)$$

$$+((y_{id}+2/r_1)e^{-y_{id}r_1} + (x_{id}+2/r_1)e^{-x_{id}r_1} - (y_{id}+2/r_p)e^{-y_{id}r_p}$$

$$-(x_{id}+2/r_p)e^{-x_{id}r_p} + \Delta(\; x_{id}(1-x_i) + (2-y_i)y_{id} + x_i^2 + y_i^2 + E_{He}$$

$$+(y_{id}(x_{id})^3/(x_{id}+y_{id})^3+x_{id}^3)/(x_{id}+y_{id})^2))$$

$$x\ J_o(1-2\beta,2\gamma,r_1,q_j+q_k,m_j+m_k))dr_1dr_p \qquad .....(B.30)$$

The exchange term becomes

$$K_{jk})_{exchange} = 0.5\int\phi_1\phi_2\psi_{23}\chi_j^{(1)}\chi_k^{(2)}N_1\sum_{i=1}^{M}u_i e^{-x_i r_1}e^{-y_i r_3}$$

$$x(q_k(q_k+1)/r_2^2 +(4-2\gamma(q_k+1))/r_2+\gamma^2+h_k(h_k+1)/r_p^2 +\eta^2+2\beta^2-2\beta$$

$$+2m_k(m_k+1)/|\vec{r}_2-\vec{r}_p|^2+2(-m_k+2\beta(m_k+1))/|\vec{r}_2-\vec{r}_p|+2/|\vec{r}_3-\vec{r}_p|$$

$$-(4+2\eta(h_k+1))/r_p+2/|\vec{r}_1-\vec{r}_p|-2/|\vec{r}_1-\vec{r}_2|-2/|\vec{r}_2-\vec{r}_3|$$

$$+(q_k/r_2-\gamma)(2m_k/|\vec{r}_2-\vec{r}_p|-1+2\beta)\vec{r}_2\cdot(\vec{r}_2-\vec{r}_p)/r_2|\vec{r}_2-\vec{r}_p|$$

$$-(h_k/r_p-\eta)(2m_k/|\vec{r}_2-\vec{r}_p|-1+2\beta)\vec{r}_p\cdot(\vec{r}_2-\vec{r}_p)/r_p|\vec{r}_2-\vec{r}_p|$$

$$+\Delta((4-2x_i)/r_1+(4-2y_i)/r_3+x_i^2+y_i^2+E_{He}-2/|\vec{r}_1-\vec{r}_3|))d\tau$$

$$+0.5\int\phi_1\phi_2\psi_{13}\chi_k^{(1)}\chi_j^{(2)}N_1\sum_{i=1}^{M}u_i e^{-x_i r_1}e^{-y_i r_3}(q_j(q_j+1)/r_2^2$$

$$+(4-2\gamma(q_j+1)/r_2+\gamma^2+h_j(h_j+1)/r_p^2-(4+2\eta(h_j+1))/r_p+\eta^2$$

$$+2m_j(m_j+1)/|\vec{r}_2-\vec{r}_p|^2+2(-m_j+2\beta(m_j+1))/|\vec{r}_2-\vec{r}_p|+2\beta^2-2\beta$$

$$+(q_j/r_2-\gamma)(2m_j/|\vec{r}_2-\vec{r}_p|-1+2\beta)\vec{r}_2\cdot(\vec{r}_2-\vec{r}_p)/r_2|\vec{r}_2-\vec{r}_p|$$

$$-(h_j/r_p-\eta)(2m_j/|\vec{r}_2-\vec{r}_p|-1+2\beta)\vec{r}_p\cdot(\vec{r}_2-\vec{r}_p)/r_p|\vec{r}_2-\vec{r}_p|$$

$$+2/|\vec{r}_1-\vec{r}_p|+2/|\vec{r}_3-\vec{r}_p|-2/|\vec{r}_1-\vec{r}_2|-2/|\vec{r}_2-\vec{r}_3|+\Delta((4-2x_i)/r_1$$

$$+(4-2y_i)/r_3 +x_i^2+y_i^2+E_{He}+2/|\vec{r}_1-\vec{r}_3|))d\tau$$

$$= 4N_1^2\pi^3 \int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d r_p^{h_j+h_k} e^{-2\eta r_p} \left(\frac{8}{y_{id}}\right)^3 r_1 r_2$$

$$x(J_o(0.5-\beta,\gamma+x_i,r_1,q_j,m_j)(J_o(0.5-\beta,\gamma+x_d,r_2,q_k,m_k)(2/r_2$$

$$+(y_{id}+2/r_2)e^{-y_{id}r_2}-2/r_p-(y_{id}+2/r_p)e^{-y_{id}r_p}+\Delta(y_{id}(2-y_i)+x_i^2$$

$$+y_i^2+E_{He}))+L(0.5-\beta,\gamma+x_d,r_2,q_k,m_k,\beta,\gamma,\eta,h_k,q_k,m_k))$$

$$+J_o(0.5-\beta,\gamma+x_d,r_2,q_k,m_k)(2J_o(0.5-\beta,\gamma+x_i,r_1,q_j,m_j-1)$$

$$+\Delta((2-2x_i)/r_1+(y_{id}+2/r_1)e^{-y_{id}r_1})J_o(0.5-\beta,\gamma+x_i,r_1,q_j,m_j))$$

$$-2\sum_{\ell=0}^{\infty} J_\ell(0.5-\beta,\gamma+x_i,r_1,q_j,m_j)J_\ell(0.5-\beta,\gamma+x_d,r_2,q_k,m_k)$$

$$x\ \gamma_\ell(r_1,r_2))\ \ dr_2 dr_p dr_1$$

$$+4N_1^2\pi^3 \int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d r_p^{h_j+h_k} e^{-2\eta r_p} \left(\frac{8}{y_{id}}\right)^3 r_1 r_2$$

$$x(J_o(0.5-\beta,\gamma+x_i,r_1,q_k,m_k)(J_o(0.5-\beta,\gamma+x_d,r_2,q_j,m_j)(2/r_2$$

$$+(y_{id}+2/r_2)e^{-y_{id}r_2}-2/r_p-(y_{id}+2/r_p)e^{-y_{id}r_p}+\Delta(y_{id}(2-y_i)+x_i^2$$

$$+y_i^2+E_{He}))+L(0.5-\beta,\gamma+x_d,r_2,q_j,m_j,\beta,\gamma,\eta,h_j,q_j,m_j))$$

$$+J_o(0.5-\beta,\gamma+x_d,r_2,q_j,m_j)(2J_o(0.5-\beta,\gamma+x_i,r_1,q_k,m_k-1)$$

$$+\Delta((2-2x_i)/r_1+(y_{id}+2/r_1)e^{-y_{id}r_1})J_o(0.5-\beta,\gamma+x_i,r_1,q_k,m_k))$$

$$-2\sum_{\ell=0}^{\infty} J_\ell(0.5-\beta,\gamma+x_i,r_1,q_k,m_k)J_\ell(0.5-\beta,\gamma+x_d,r_2,q_j,m_j)$$

$$x\ \gamma_\ell(r_1,r_2))\ \ dr_2 dr_p dr_1 \qquad \text{.....(B.31)}$$

(b) Effective Charge

A similar analysis to that given for the scattering length may be applied to the effective charge calculations.

$$A' = \{v/\sigma, v/\sigma\} = \int \phi_2^2 \psi_{13}^2 (v_2^2/\sigma_2^2) d\tau \Big|_{\vec{r}_p = \vec{r}_1}$$

$$- \int \phi_2 \phi_3 \psi_{12} \psi_{13} (v_2/\sigma_2)(v_3/\sigma_3) d\tau \Big|_{\vec{r}_p = \vec{r}_1}$$

Here the direct term (that is, the first term in the above expression) is given by

$$A')_{\text{direct}} = 1 \qquad \text{.....(B.32)}$$

since the wavefunctions are normalized.

The exchange term (that is, the second term in the equation for A') is

$$A')_{\text{exchange}} = -\frac{N_1^2}{8\pi} \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d e^{-y_{id} r_p} \, e^{-x_i |2\vec{\sigma}_3 - \vec{r}_p|}$$

$$e^{-|\vec{\sigma}_3 - \vec{r}_p|} e^{-|\vec{\sigma}_2 - \vec{r}_p|} e^{-x_d |2\vec{\sigma}_2 - \vec{r}_p|} (v_2/\sigma_2)(v_3/\sigma_3) 64 d\vec{\sigma}_2 d\vec{\sigma}_3 d\vec{r}_p$$

$$= -512 N^2 \pi^3 \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d e^{-y_{id} r_p} \, v_2 v_3 G_o(1, x_d, \sigma_2, 0, 0)$$

$$\times \, G_o(1, x_i, \sigma_3, 0, 0) d\sigma_2 d\sigma_3 dr_p \qquad \text{.....(B.33)}$$

$$B' = 2\{v/\sigma, w/\sigma\} = 2 \int \phi_2^2 \psi_{13}^2 (v_2 w_2/\sigma_2^2) d\tau \Big|_{\vec{r}_p = \vec{r}_1}$$

$$-2\int \phi_2\phi_3\psi_{12}\psi_{23}(v_2/\sigma_2)(w_3/\sigma_3)d\tau\Big|_{\vec{r}_p=\vec{r}_1}$$

Here $B')_{direct} = (N_1^2/8\pi)\int \sum_{\substack{i=1\\d=1}}^{M} u_i u_d \frac{8\pi}{(y_{id})^3}(v_2 w_2/\sigma_2^2)e^{-\rho_2}$

$$x\ e^{-0.5x_{id}|\vec{\rho}_2-2\vec{\sigma}_2|}\,d\vec{\sigma}_2\,d\vec{\rho}_2$$

$$= -N_1^2\int \sum_{\substack{i=1\\d=1}}^{M} (1/(y_{id})^3)(8\pi/(1-0.25x_{id}^2)^2(0.5x_{id}e^{-2\sigma_2}+e^{-x_{id}\sigma_2}$$

$$+2x_{id}/(2\sigma_2(1-0.25x_{id}^2))(e^{-2\sigma_2}-e^{-x_{id}\sigma_2})))4\pi\sigma_2^2 d\sigma_2$$

using equation (A.5) . $B')_{direct}$ further reduces to

$$B')_{direct} = -8\pi^2 N_1^2 \sum_{\substack{i=1\\d=1}}^{M} u_i u_d \frac{8}{(y_{id})^3}(1/(1-0.25x_{id}^2)^2)(0.125x_{id}$$

$$-x_{id}0.5/(2+\delta)^2+1/x_{id}^2-1/(x_{id}+\delta)^2+x_{id}/(1-0.25x_{id}^2)(0.5$$

$$-1/(2+\delta)-1/x_{id}+1/(x_{id}+\delta))) \qquad .....(B.34)$$

$B')_{exchange}$ is the same as that given for $A')_{exchange}$ in equation (B.33) replacing $(v_2v_3/\sigma_2\sigma_3)$ by $2v_2w_3/\sigma_2\sigma_3$.

$$C' = \{w/\sigma, w/\sigma\} = \int \phi_2^2\psi_{13}^2(w_2^2/\sigma_2^2)d\tau\Big|_{\vec{r}_p=\vec{r}_1}$$

$$-\int \phi_2\phi_3\psi_{12}\psi_{13}(w_2w_3/\sigma_2\sigma_3)d\tau\Big|_{\vec{r}_p=\vec{r}_1}$$

Here $C')_{direct}$ reduces to

$$C')_{direct} = 4\pi^2N^2\sum_{i=1}^{M}\sum_{d=1}^{1} u_i u_d \left(\frac{8}{y_{id}}\right)^3 (1/(1-0.25x_{id}^2)^2(0.25x_{id}$$

$$-x_{id}/(2+\delta)+x_{id}/(4+4\delta)+1/x_{id}-2/(x_{id}+\delta)+1/(x_{id}+2\delta)$$

$$+x_{id}/(1-0.25x_{id}^2)(\log(0.5x_{id})-2\log((x_{id}+\delta)/(2+\delta))$$

$$+\log((x_{id}+2\delta)/(2+2\delta)))) \qquad \text{.....(B.35)}$$

$C')_{exchange}$ is the same as that given for $A')_{exchange}$ in equation (B.33) replacing $v_2v_3\ \sigma_2\sigma_3$ by $w_2w_3/\sigma_2\sigma_3$.

$$D_k' = 2\{v/\sigma, h_k/\sigma\} = 2\int \phi_2^2\psi_{13}^2 (v_2 h_k^{(2)}/\sigma_2^2)d\tau\Big|_{\vec{r}_p=\vec{r}_1}$$

$$-2\int \phi_2\phi_3\psi_{12}\psi_{13}(v_2 h_k^{(3)}/\sigma_2\sigma_3)d\tau\Big|_{\vec{r}_p=\vec{r}_1}$$

Here $D')_{direct}$ reduces to

$$D_k')_{direct} = -8\pi^2N^2\sum_{i=1}^{M}\sum_{d=1}^{1} u_i u_d \left(\frac{8}{y_{id}}\right)^3 (1/(1-0.25x_{id}^2)^2)\ k!$$

$$x((x_{id}(k+1)0.5/(2+\delta)^{k+2})+(k+1)/(x_{id}+\delta)^{k+2}$$

$$+x_{id}/(1-0.25x_{id}^2)(1/(2+\delta)^{k+1} - 1/(x_{id}+\delta)^{k+1}))$$

$$\text{.....(B.36)}$$

$D_k')_{exchange}$ is the same as that given for $A')_{exchange}$ in equation (B.33) replacing $v_2v_3/\sigma_2\sigma_3$ by $2v_2h_k^{(3)}/\sigma_2\sigma_3$.

$$E'_k = 2\{w/\sigma, h_k/\sigma\} = 2\int \phi_2^2 \psi_{13}^2 (w_2 h_k^{(2)}/\sigma_2^2) d\tau \Big|_{\vec{r}_p=\vec{r}_1}$$

$$-2\int \phi_2 \phi_3 \psi_{12} \psi_{13} (w_2 h_k^{(3)}/\sigma_2 \sigma_3) d\tau \Big|_{\vec{r}_p=\vec{r}_1}$$

Here $E'_{k)\,direct}$ reduces to

$$E'_{k)\,direct} = 8\pi^2 N^2 \sum_{i=1}^{M} \sum_{d=1} u_i u_d \left(\frac{8}{y_{id}}\right)^3 (1/(1-0.25x_{id}^2)\ (k-1)!(k$$

$$x(0.5x_{id}/(2+\delta)^{k+1} - 0.5x_{id}/(2+2\delta)^{k+1} + 1/(x_{id}+\delta)^{k+1}$$

$$-1/(x_{id}+2\delta)^{k+1}) + (x_{id}/(1-0.25x_{id}^2))(1/(2+\delta)^k - 1/(2+2\delta)^k$$

$$-1/(x_{id}+\delta)^k + 1/(x_{id}+2\delta)^k))) \qquad .....(B.37)$$

$E'_{k)\,exchange}$ is the same as that given for $A'_{)\,exchange}$ in equation (B.33) replacing $v_2 v_3/\sigma_2\sigma_3$ by $2w_2 h_k^{(3)}/\sigma_2\sigma_3$.

$$F'_{jk} = \{h_j/\sigma, h_k/\sigma\}$$

Here $F'_{jk)\,direct}$ reduces to

$$F'_{jk)\,direct} = 4\pi^2 N^2 \sum_{i=1}^{M} \sum_{d=1} u_i u_d \left(\frac{8}{y_{id}}\right)^3 (1/(1-0.25x_{id}^2)\ (j+k-1)!$$

$$x((j+k)(x_{id}0.5/(2+2\delta)^{j+k+1} + 1/(x_{id}+2\delta)^{j+k+1}$$

$$+(x_{id}/(1-0.25x_{id}^2))(1/(2+2\delta)^{j+k} - 1/(x_{id}+2\delta)^{j+k})))$$

.....(B.38)

$F'_{jk})_{\text{exchange}}$ is the same as that given for $A')_{\text{exchange}}$ in equation (B.33) replacing $v_2 v_3/\sigma_2\sigma_3$ by $h_j^{(2)}h_k^{(3)}/\sigma_2\sigma_3$.

$$R'_k = 2\{v/\sigma, \chi_k\}$$

Here

$$R'_k)_{\text{direct}} = 32\pi^2 N_1^2 \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d \left(\frac{8}{y_{id}}\right)^3 e^{-(x_{id}+\eta)r_p} r_p^{h_k+1} v_2$$

$$x\ G_o(2-2\beta, \gamma, \sigma_2, q_k, m_k)d\sigma_2 dr_p \qquad .....(B.39)$$

$$R'_k)_{\text{exchange}} = -128\pi^2 N_1^2 \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d e^{-(y_{id}+\eta)r_p} r_p^{h_k} v_2$$

$$x\ Go(1, x_d, \sigma_2, 0, 0)J_o(0.5-\beta, x_i+\gamma, r_3, q_k, m_k)d\sigma_2 dr_3 dr_p$$

.....(B.40)

$$H'_k = 2\{w/\sigma, \chi_k\}$$

$$S'_{jk} = 2\{h_j/\sigma, \chi_k\}$$

Here $H'_k)_{\text{direct}}$ and $S'_{jk})_{\text{direct}}$ are the same as that given by $R'_k)_{\text{direct}}$ in equation (B.39) replacing v_2 by w_2 and $h_j^{(2)}$ respectively. Similarly, $H'_k)_{\text{exchange}}$ and $S'_{jk})_{\text{exchange}}$ are the same as that given by $R'_k)_{\text{exchange}}$ replacing v_2 by w_2 and $h_j^{(2)}$ respectively.

$$K'_{jk} = \{\chi_j, \chi_k\}$$

Here

$$K'_{jk})_{direct} = 2\pi^2 N_1^2 \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d \frac{8}{(y_{id})^3} e^{-(x_{id}+2\eta)r_p} r_2$$

$$x\ r_p^{h_j+h_k+1}\ J_o(1-2\beta, 2\gamma, r_2, q_j+q_k, m_j+m_k) dr_2 dr_p \qquad .....(B.41)$$

$$K'_{jk})_{exchange} = -8\pi^2 N_1^2 \int \sum_{\substack{i=1 \\ d=1}}^{M} u_i u_d r_2 r_3 r_p^{h_j+h_k}\ e^{-(y_{id}+2\eta)r_p}$$

$$xJ_o(0.5-\beta, x_d+\gamma, r_2, q_j, m_j) J_o(0.5-\beta, x_i+\gamma, r_3, q_k, m_k)$$

$$x dr_2 dr_3 dr_p \qquad .....(B.42)$$

(c) Hylleraas He Ground State Wavefunction

Using the simple Hylleraas He ground state wavefunction defined by equation (3.40), equation (B.3) becomes

$$A)_{exchange} = 512\mu^3\pi \int v_1 v_2 (G_o(1, \mu, \sigma_1, 0, 0)(-2/r_p$$

$$-(2\mu + 2/r_p)e^{-2\mu r_p}) G_o(1, \mu, \sigma_2, 0, 0) + 2G_o(1, \mu, \sigma_2, -1, 0)$$

$$+ 2\mu G_o(1, 3\mu, \sigma_2, 0, 0) + 2G_o(1, 3\mu, \sigma_2, -1, 0))$$

$$+ G_o(1, \mu, \sigma_2, 0, 0)(G_o(1, \mu, \sigma_1, 0, -1) + \Delta(\mu(4-2\mu)$$

$$x\ G_o(1, \mu, \sigma_1, 0, 0) + (2-2\mu)G_o(1, \mu, \sigma_1, -1, 0)$$

$$+2\mu G_o(1,3\mu,\sigma_1,0,0) + 2G_o(1,3\mu,\sigma_1,-1,0)))$$

$$-\sum_{\ell=0}^{\infty} G_\ell(1,\mu,\sigma_1,0,0)G_\ell(1,\mu,\sigma_2,0,0)\gamma_\ell(\sigma_1,\sigma_2))\ d\sigma_2 dr_p d\sigma_1 \qquad \text{.....(B.41)}$$

Similar expressions may be obtained for all the other quantities developed in Section B.1.

(d) Hartree-Fock Type He Ground State Wavefunction

Using the Hartree-Fock type He ground state wavefunction defined by equation (3.42), equation (B.3) becomes

$$A)_{\text{exchange}} = (64\pi/DK)\int v_1 v_2((G_o(1,\lambda,\sigma_1,0,0)$$

$$+N_3 G_o(1,2\lambda,\sigma_1,0,0))(-2/r_p-(1/DK)((2\lambda+2/r_p)e^{-2\lambda r_p}/(8\lambda^3)$$

$$+(2N_3/27\lambda^3)(3\lambda+2/r_p)e^{-3\lambda r_p} +(N_3^2/64\lambda^3)(4\lambda+2/r_p)e^{-4\lambda r_p))$$

$$x(G_o(1,\lambda,\sigma_2,0,0)+N_3 G_o(1,2\lambda,\sigma_2,0,0))+2(G_o(1,\lambda,\sigma_2,-1,0)$$

$$+N_3 G_o(1,2\lambda,\sigma_2,-1,0))+(1/DK)((1/8\lambda^3)(2\lambda(G_o(1,3\lambda,\sigma_2,0,0)$$

$$+N_3 G_o(1,4\lambda,\sigma_2,0,0))+2(Go(1,3\lambda,\sigma_2,-1,0)+N_3$$

$$xG_o(1,4\lambda,\sigma_2,-1,0))+(2N_3/27\lambda^3)(3\lambda(G_o(1,4\lambda,\sigma_2,0,0)$$

$$+N_3 G_o(1,5\lambda,\sigma_2,0,0)+2(G_o(1,4\lambda,\sigma_2,-1,0)+N_3$$

$$xG_o(1,5\lambda,\sigma_2,-1,0)))+(N_3^2/64\lambda^3)(4\lambda(G_o(1,5\lambda,\sigma_2,0,0)$$

$$+N_3 G_o(1,6\lambda,\sigma_2,0,0))+2(G_o(1,5\lambda,\sigma_2,-1,0)+N_3$$

$$xG_o(1,6\lambda,\sigma_2,-1,0))))+(G_o(1,\lambda,\sigma_2,0,0)+N_3G_o(1,2\lambda,\sigma_2,0,0))$$

$$x(G_o(1,\lambda,\sigma_1,0,-1)+N_3G_o(1,2\lambda,\sigma_1,0,-1)+\Delta(2(G_o(1,\lambda,\sigma_1,-1,0)$$

$$+N_3G_o(1,2\lambda,\sigma_1,-1,0))-2\lambda(G_o(1,\lambda,\sigma_1,-1,0)+2N_3$$

$$xG_o(1,2\lambda,\sigma_1,-1,0))+\lambda^2(G_o(1,\lambda,\sigma_1,0,0)+4N_3G_o(1,2\lambda,\sigma_1,0,0))$$

$$+((1/DK)((\lambda^2(1/8\lambda^3+N_3/27\lambda^3)+4\lambda^2(N_3/27\lambda^3+N_3^2/64\lambda^3)$$

$$+2\lambda(2-\lambda)/8\lambda^3+3\lambda(2-\lambda)N_3/27\lambda^3+3\lambda(2-2\lambda)N_3/27\lambda^3$$

$$+4\lambda(2-2\lambda)N_3^2/64\lambda^3))+E_{He})(G_o(1,\lambda,\sigma_1,0,0)+N_3$$

$$xG_o(1,2\lambda,\sigma_1,0,0))+(1/DK)((1/8\lambda^3)(2\lambda(G_o(1,3\lambda,\sigma_1,0,0)$$

$$+N_3G_o(1,4\lambda,\sigma_1,0,0))+2(G_o(1,3\lambda,\sigma_1,-1,0)+N_3$$

$$xG_o(1,4\lambda,\sigma_1,-1,0)))+(2N_3/27\lambda^3)(3\lambda(G_o(1,4\lambda,\sigma_1,0,0)$$

$$+N_3G_o(1,5\lambda,\sigma_1,0,0)+2(G_o(1,4\lambda,\sigma_1,-1,0)+N_3$$

$$xG_o(1,5\lambda,\sigma_1,-1,0)))+(N_3^2/64\lambda^3)(4\lambda(G_o(1,5\lambda,\sigma_1,0,0)$$

$$+N_3G_o(1,6\lambda,\sigma_1,0,0))+2(G_o(1,5\lambda,\sigma_1,-1,0)+N_3$$

$$xG_o(1,6\lambda,\sigma_1,-1,0)))))) - \sum_{\ell=0}^{\infty} \gamma_\ell(\sigma_1,\sigma_2)(G_\ell(1,\lambda,\sigma_1,0,0)$$

$$+N_3G_\ell(1,2\lambda,\sigma_1,0,0))(G_\ell(1,\lambda,\sigma_2,0,0)+N_3G_\ell(1,2\lambda,\sigma_2,0,0)))$$

$$xd\sigma_1d\sigma_2dr_p \qquad \text{.....(B.42)}$$

Here

$$DK = 1/8\lambda^3+2N_3/27\lambda^3+N_3^2/64\lambda^3 = 25.21/144\lambda^3$$

and $E_{H_e} = -5.72334$ with $N_3 = 0.6$.

Similar expressions may be obtained for all the other quantities developed in Section B.1.

B.2 Ps-H System

Expressions for the quantities defined by equations (3.11) through to (3.20) in terms of the functions G_ℓ and J_ℓ may be determined in a similar fashion to those given in Section B.1. For convenience, only the antisymmetric case is given. The symmetric case corresponds to a change of sign of the exchange term in all of the quantities given below.

$$A = (v/\sigma, v/\sigma) = \int \phi_1 \psi_2 (v_1/\sigma_1)(H-E)\phi_1 \psi_2 (v_1/\sigma_1)d\tau$$

$$-\int \phi_1 \psi_2 (v_1/\sigma_1)(H-E)\phi_2 \psi_1 (v_2/\sigma_2)d\tau \qquad .....(B.43)$$

Here

$$A)_{\text{direct}} = 0 \qquad .....(B.44)$$

and

$$A)_{\text{exchange}} = 512\pi \int v_1 v_2 (G_o(1,1,\sigma_1,0,0)((-2/r_p)$$

$$xG_o(1,1,\sigma_2,0,0)+2G_o(1,1,\sigma_2,-1,0))+G_o(1,1,\sigma_2,0,0)$$

$$xG_o(1,1,\sigma_1,0,-1) - \sum_{\ell=0}^{\infty} G_\ell(1,1,\sigma_1,0,0)G_\ell(1,1,\sigma_2,0,0)$$

$$x\gamma_\ell(\sigma_1,\sigma_2))d\sigma_1 d\sigma_2 dr_p \qquad .....(B.45)$$

$$B = (v/\sigma, w/\sigma) + (w/\sigma, v/\sigma) \qquad \text{.....(B.46)}$$

Here

$$B)_{\text{direct}} = -2\pi \qquad \text{.....(B.47)}$$

The exchange term is the same as that given for $A)_{\text{exchange}}$ in equation (B.45) replacing the product $v_1 v_2$ by $(v_1 w_2 + v_2 w_1)$ with the addition of the term

$$-256\pi \int v_1 (\delta^2 e^{-\delta\sigma_2}) G_o(1,1,\sigma_1,0,0) G_o(1,1,\sigma_2,0,0) d\sigma_1 d\sigma_2 dr_p \qquad \text{.....(B.48)}$$

$$C = (w/\sigma, w/\sigma) \qquad \text{.....(B.49)}$$

Here

$$C)_{\text{direct}} = \pi\delta \qquad \text{.....(B.50)}$$

The exchange term is the same as that given for $A)_{\text{exchange}}$ in equation (B.45) replacing $v_1 v_2$ by $w_1 w_2$ with the additional term given by equation (B.48) replacing v_1 by w_1 being added.

$$D_k = 2(v/\sigma, h_k/\sigma) \qquad \text{.....(B.51)}$$

Here

$$D_k)_{\text{direct}} = 0 \qquad \text{.....(B.52)}$$

The exchange term is the same as that given for $A)_{exchange}$ in equation (B.45) replacing $v_1 v_2$ by $2v_1 h_k^{(2)}$.

$$E_k = 2(w/\sigma, h_k/\sigma) \qquad \text{.....(B.53)}$$

Here

$$E_k)_{direct} = \pi k!/(2\delta)^{k-1} \qquad \text{.....(B.54)}$$

The exchange term is the same as that given for $A)_{exchange}$ in equation (B.45) replacing $v_1 v_2$ by $2w_1 h_k^{(2)}$ with the additional term given by equation (B.48) replacing v_1 by $h_k^{(1)}$ being added on.

$$F_{jk} = (h_j/\sigma, h_k/\sigma) \qquad \text{.....(B.55)}$$

Here

$$F_{jk})_{direct} = -2\pi(-jk + 0.25(j+k)(j+k-1))(j+k-2)!/(2\delta)^{j+k} \times (2\delta) \qquad \text{.....(B.56)}$$

The exchange term is the same as that given for $A)_{exchange}$ in equation (B.45) replacing $v_1 v_2$ by $h_j^{(1)} h_k^{(2)}$ with the addition of the term

$$256\pi \int h_j^{(1)} (k(k-1)/\sigma_2^2 - 2k\delta/\sigma_2 + \delta^2)\sigma_2^k e^{-\delta\sigma_2} G_o(1,1,\sigma_1,0,0) \times G_o(1,1,\sigma_2,0,0) d\sigma_1 d\sigma_2 dr_p \qquad \text{.....(B.57)}$$

$$R_k = 2(v/\sigma, \chi_k) \qquad \text{.....(B.58)}$$

Here the direct term reduces to

$$R_k)_{\text{direct}} = -2\int \phi_1^2 \psi_2^2 (v_1/\sigma_1) \chi_k^{(1)} (q_k(q_k+1)/r_1^2 - 2\gamma(q_k+1)/r_1 + \gamma^2$$

$$+2(q_k/r_1 - \gamma)(m_k/|\vec{r}_1 - \vec{r}_p| + \beta - 0.5)\vec{r}_1 \cdot (\vec{r}_1 - \vec{r}_p)/r_1 |\vec{r}_1 - \vec{r}_p| + 2\beta^2$$

$$+2m_k(m_k+1)/|\vec{r}_1 - \vec{r}_p|^2 + 2(-m_k + 2\beta(m_k+1))/|\vec{r}_1 - \vec{r}_p| - 2\beta + \eta^2 + 2/r_1$$

$$-(h_k/r_p - \eta)(2m_k/|\vec{r}_1 - \vec{r}_p| - 1 + 2\beta)\vec{r}_p \cdot (\vec{r}_1 - \vec{r}_p)/r_p |\vec{r}_1 - \vec{r}_p| - 2/r_p$$

$$+h_k(h_k+1)/r_p^2 - 2\eta(h_k+1)/r_p + 2/|r_2 - r_p| - 2/|\vec{r}_1 - \vec{r}_2|)d\tau$$

$$= -32\pi \int r_p^{h_k+1} e^{-\eta r_p} v_1 (Q(2-2\beta, \gamma, \sigma_1, q_k, m_k, \beta, \gamma, \eta, h_k, q_k, m_k)$$

$$+2G_o(2-2\beta, \gamma+2, \sigma_1, q_k-1, m_k) + 2G_o(2-2\beta, \gamma+2, \sigma_1, q_k, m_k)$$

$$-(2+2/r_p)e^{-2r_p} G_o(2-2\beta, \gamma, \sigma_1, q_k, m_k) d\sigma_1 dr_p \qquad \text{.....(B.59)}$$

Similarly, the exchange term reduces to

$$R_k)_{\text{exchange}} = 2\int \phi_1 \phi_2 \psi_1 \psi_2 (v_1/\sigma_1) \chi_k^{(2)} (q_k(q_k+1)/r_2^2 + \gamma^2 + \eta^2$$

$$+(2 - 2\gamma(q_k+1))/r_2 + 2(q_k/r_2 - \gamma)(m_k/|\vec{r}_2 - \vec{r}_p| + -0.5)\vec{r}_2 \cdot (\vec{r}_2 - \vec{r}_p)$$

$$/r_2 |\vec{r}_2 - \vec{r}_p| + 2m_k(m_k+1)/|\vec{r}_2 - \vec{r}_p|^2 + 2(-m_k + 2\beta(m_k+1))/|\vec{r}_2 - \vec{r}_p|$$

$$+h_k(h_k+1)/r_p^2 - 2\eta(h_k+1)/r_p - 2/r_p + 2/|\vec{r}_1 - \vec{r}_p| - 2/|\vec{r}_1 - \vec{r}_2|$$

$$-(h_k/r_p - \eta)(2m_k/|\vec{r}_2 - \vec{r}_p| - 1 + 2\beta)\vec{r}_p \cdot (\vec{r}_2 - \vec{r}_p)/r_p |\vec{r}_2 - \vec{r}_p|)d\tau$$

$$= 128\pi\int v_1 r_2 r_p^{h_k} e^{-\eta r_p}(G_o(1,1,\sigma_1,0,0)((2/r_2-2/r_p)$$

$$xJ_o(0.5-\beta,1+\gamma,r_2,q_k,m_k)+L(0.5-\beta,1+\gamma,r_2,q_k,m_k,\beta,\gamma,\eta,h_k,$$

$$q_k,m_k))+J_o(0.5-\beta,1+\gamma,r_2,q_k,m_k)G_o(1,1,\sigma_1,0,-1)d\sigma_1 dr_2 dr_p$$

$$-1024\pi\int \sum_{\ell=0}^{\infty} G_\ell(1,1,\sigma_1,0,0)G_\ell(1-2\beta,1+\gamma,\sigma_2,q_k,m_k)$$

$$x\,\gamma_\ell(\sigma_1,\sigma_2)d\sigma_1 d\sigma_2 dr_p) \qquad .....(B.60)$$

$$H_k = 2(w/\sigma,\chi_k) = 2(\chi_k,w/\sigma) \qquad .....(B.61)$$

$$S_{jk} = 2(h_j/\sigma,\chi_k) = 2(\chi_k,h_j/\sigma) \qquad .....(B.62)$$

Here $H_k)_{direct}$ and $S_{jk})_{direct}$ are the same as that given for $R_k)_{direct}$ in equation (B.59) replacing v_1 by w_1 and $h_j^{(1)}$ respectively. Similarly, $H_k)_{exchange}$ and $S_{jk})_{exchange}$ are the same as that given for $R_k)_{exchange}$ in equation (B.60) replacing v_1 by w_1 and $h_j^{(1)}$ respectively.

$$K_{jk} = (\chi_j,\chi_k) \qquad .....(B.63)$$

Here

$$K_{jk})_{direct} = -2\pi\int r_p^{h_j+h_k+1} e^{-2\eta r_p} r_1(((2+2/r_1)e^{-2r_1}-(2+$$

$$2/r_p)e^{-2r_p})J_o(1-2\beta,2\gamma,r_1,q_j+q_k,m_j+m_k)$$

$$+L(1-2\beta,2\gamma,r_1,q_j+q_k,m_j+m_k,\beta,\gamma,\eta,h_k,q_k,m_k))dr_1dr_p$$

.....(B.64)

$$K_{jk})_{\text{exchange}} = 8\pi\int r_p^{h_j+h_k}\, e^{-2\eta r_p}\, r_1 r_2 (J_o(0.5-\beta,1+\gamma,r_1,q_j$$

$$,m_j)(L(0.5-\beta,1+\gamma,r_2,q_k,m_k,\beta,\gamma,\eta,h_k,q_k,m_k)+(2/r_2-2/r_p)$$

$$x\ J_o(0.5-\beta,1+\gamma,r_2,q_k,m_k))+J_o(0.5-\beta,1+\gamma,r_2,q_k,m_k)$$

$$x\ J_o(0.5-\beta,1+\gamma,r_1,q_j,m_j-1)-2\sum_{\ell=0}^{\infty} J_\ell(0.5-\beta,1+\gamma,r_1,q_j,m_j)$$

$$x\ J_\ell(0.5-\beta,1+\gamma,r_2,q_k,m_k)\ \gamma_\ell(r_1,r_2))\ \ dr_2dr_pdr_1$$

.....(B.65)

APPENDIX C

NUMERICAL TECHNIQUES

In evaluating integrals containg G_ℓ, inaccuracies may occur due to the presence of the radicals $|\vec{\sigma} - \vec{r}_p|$ and $|2\vec{\sigma} - \vec{r}_p|$. This difficulty may be overcome by two changes of variable for different regions of the (σ, r_p) quadrant (Fraser (1962)). Here

$$\mu = \vec{\sigma}\cdot\vec{r}_p/(\sigma r_p) \ , \ -1 \leq \xi \leq 1 \ , \ p=r_p/\sigma, \ q=2\sigma/r_p \qquad .....(C.1)$$

Region 1:

$$0 \leq p \leq 1, \ \mu = p/2-\xi-p\xi^2/2, \ |\vec{\sigma}-\vec{r}_p| = \sigma(1+p\xi),$$

$$|2\vec{\sigma}-\vec{r}_p| = \sigma(2(1+p\xi)^2+2-p^2)^{\frac{1}{2}} = \sigma x SQ1 \qquad .....(C.2)$$

Region 2:

$$1 \leq p \leq (2)^{\frac{1}{2}} \ , \ \mu = 0.5/p-\xi-0.5\xi^2/p, \ |\vec{\sigma}-\vec{r}_p| = \sigma(p+\xi),$$

$$|2\vec{\sigma}-\vec{r}_p| = \sigma(2(p+\xi)^2+2-p^2)^{\frac{1}{2}} = \sigma x SQ2 \qquad .....(C.3)$$

Region 3:

$$0 \leq q \leq 1, \ \mu = q/2-\xi-q\xi^2/2, \ |2\vec{\sigma}-\vec{r}_p| = r_p(1+q\xi),$$

$$|\vec{\sigma}-\vec{r}_p| = 0.5r_p(2(1+q\xi)^2+2-q^2)^{\frac{1}{2}} = 0.5r_p SQ3 \qquad .....(C.4)$$

Region 4:

$$1 \leq q \leq (2)^{\frac{1}{2}}\ ,\ \mu = 0.5/q-\xi-0.5\xi^2/q,\ |2\vec{\sigma}-\vec{r}_p| = r_p(q+\xi),$$

$$|\vec{\sigma}-\vec{r}_p| = 0.5r_p(2(q+\xi)^2+2-q^2)^{\frac{1}{2}} = r_p 0.5SQ4 \qquad \text{.....(C.5)}$$

With these changes of variable, the function $G_{\ell}(\alpha,\beta,\sigma,m,n)$ defined by (A.9) becomes

Region 1: $0 \leq p \leq 1$

$$G_{\ell}(\alpha,\beta,\sigma,m,n) = 0.5\sigma r_p \int_{-1}^{1} d\xi (1+p\xi)^{n+1}\ \sigma^{n+m}\ (SQ1)^m$$

$$\times\ P_{\ell}(p/2-\xi-p\xi^2/2) e^{-\sigma(\alpha(1+p\xi)+\beta SQ1)} \qquad \text{.....(C.6)}$$

Region 2: $1 \leq p \leq (2)^{\frac{1}{2}}$

$$G\ell(\alpha,\beta,\sigma,m,n) = 0.5\sigma^2 \int_{-1}^{1} d\xi (p+\xi)^{n+1}\ \sigma^{m+n}\ (SQ2)^m$$

$$\times\ P_{\ell}(0.5/p-\xi-0.5\xi^2/p) e^{-\sigma(\alpha(p+\xi)+\beta SQ2)} \qquad \text{.....(C.7)}$$

Region 3: $0 \leq q \leq 1$

$$G_{\ell}(\alpha,\beta,\sigma,m,n) = 0.5\sigma r_p \int_{-1}^{1} d\xi (1+q\xi)^{m+1}\ r_p^{m+n} (0.5SQ3)^n$$

$$\times\ P_{\ell}(q/2-\xi-q\xi^2/2) e^{-r_p(0.5\alpha SQ3+\beta(1+q\xi))} \qquad \text{.....(C.8)}$$

Region 4: $1 \leq q \leq (2)^{\frac{1}{2}}$

$$G_{\ell}(\alpha,\beta,\sigma,m,n) = 0.25 r_p \int_{-1}^{1} d\xi (q+\xi)^{m+1}\ r_p^{m+n} (0.5SQ4)^n$$

$$\times\ P_{\ell}(0.5/q-\xi-0.5\xi^2/q) e^{-r_p(0.5\alpha SQ4+\beta(q+\xi))}$$

.....(C.9)

For the radial integration of the type given by equation (A.12), the following procedure is adopted. The σ-range is divided into 3 sections corresponding to

$$0 \leq \sigma \leq r_p/2 \ , \quad r_p/2 \leq \sigma \leq r_p \ , \quad r_p \leq \sigma < \infty \ .$$

Three new variables are introduced for these sections, namely

$$\sigma = r_p(x_1 + 1)/4, \qquad -1 \leq x_1 \leq 1 \qquad .....(C.10)$$

$$\sigma = r_p(x_2 + 3)/4, \qquad -1 \leq x_2 \leq 1 \qquad .....(C.11)$$

$$\sigma = r_p + x_3 \ , \qquad 0 \leq x_3 < \infty \qquad .....(C.12)$$

with

$$0 \leq r_p < \infty .$$

For integrals of the type given by equation (A.17), a slightly different procedure is adopted. Here it is only necessary to use a single change of variable for the radial integrations, namely that defined by equations (C.1), (C.2) and (C.3) with the $(2)^{\frac{1}{2}}$ in equation (C.3) being replaced by ∞. The σ_2 - range is divided into 2 sections corresponding to $0 \leq \sigma_2 \leq \sigma_1$, $\sigma_1 \leq \sigma_2 < \infty$. Two new variables are introduced for these sections, namely,

$$\sigma_2 = \sigma_1(x_1 + 1)/2, \qquad -1 \leq x_1 \leq 1 \qquad .....(C.13)$$

$$\sigma_2 = \sigma_1 + x_2 \ , \qquad 0 \leq x_2 < \infty \qquad .....(C.14)$$

with

$$0 \leq r_p \leq \infty \quad ,$$

and

$$0 \leq \sigma_1 \leq \infty \quad .$$

An analogous method is adopted for evaluating integrals containing J_ℓ . However, only the radical $|\vec{r}-\vec{r}_p|$ is present in this case. Thus the change of variable is

$$\mu = \vec{r} \cdot \vec{r}_p/(rr_p), \quad -1 \leq \xi \leq 1, \quad p = r_p/r \quad .....(C.15)$$

Region 1:

$$0 \leq p \leq 1, \ \mu = p/2-\xi-p\xi^2/2, \ |\vec{r}-\vec{r}_p| = r(1+p\xi),$$

$$J_\ell(\alpha,\beta,r,m,n) = 0.5r_p r\int_{-1}^{1} d\xi(1+p\xi)^{n+1} \ r^{m+n}$$

$$x \ P_\ell(p/2-\xi-p\xi^2/2)e^{-r(\alpha(1+p\xi)+\beta)} \quad .....(C.16)$$

Region 2:

$$1 \leq p < \infty, \quad \mu = 0.5/p-\xi-0.5\xi^2/p, \quad |\vec{r}-\vec{r}_p| = r(p+\xi),$$

$$J_\ell(\alpha,\beta,r,m,n) = 0.5r^2\int_{-1}^{1} d\xi(p+\xi)^{n+1} \ r^{m+n}$$

$$x \ P_\ell(0.5/p-\xi-0.5\xi^2/p)e^{-r(\alpha(p+\xi)+\beta)} \quad .....(C.17)$$

The r-range for all radial integrations other than those given by equation (A.21) is divided into two sections

$$0 \leq r \leq r_p \qquad \text{and} \qquad r_p \leq r < \infty.$$

Two new variables are introduced given by

$$r = r_p(x_1+1)/2 \qquad -1 \leq x_1 \leq 1 \qquad \text{.....(C.18)}$$

$$r = r_p + x_2, \qquad 0 \leq x_2 < \infty \qquad \text{.....(C.19)}$$

with

$$0 \leq r_p < \infty.$$

For integrals of the type given by equation (A.21) the r_2-range is divided into 2 sections corresponding to

$$0 \leq r_2 \leq r_1, \qquad r_1 \leq r_2 < \infty.$$

Two new variables are introduced namely:

$$r = r_1(x_1 + 1)/2, \quad -1 \leq x_1 \leq 1 \qquad \text{.....(C.20)}$$

$$r = r_1 + x_2, \quad 0 \leq x_2 < \infty \qquad \text{.....(C.21)}$$

with

$$0 \leq r_1 < \infty \quad \text{and} \quad 0 \leq r_p < \infty.$$

Gaussian quadrature methods (Stroud and Secrest (1966)) are used to evaluate the integrals. A 24-point Gauss-Legendre formula is used to carry out all integrations where the interval is (-1,1). A 32-point Gauss-Laguerre formula is used to carry out all integrations where the interval is $(0,\infty)$.

Note that an n-point Gauss-Legendre quadrature would give the exact value of the integral $\int_{-1}^{1} P_{2n-1}\, dx$ if P_{2n-1} is a polynomial in x of degree (2n-1) or less (Stroud and Secrest (1966)). Also an n-point Gauss-Laguerre quadrature would give the exact value of $\int_{o}^{\infty} P_{2n-1}\, e^{-\lambda x}\, dx$ provided P_{2n-1} is a polynomial in x of degree (2n-1) or less with $\lambda = 1$ (Stroud and Secrest (1966)). However, in the present calculations, it is very laborious and uneconomical to set $\lambda = 1$ by a scale change of variable. It has been shown that provided $1 \leq \lambda \leq 1.6$ reasonable accuracy may be achieved (Page, to be published). This property is exploited in the present calculations.

Certain methods were developed as a useful means of testing the accuracy of the integration procedures as well as the various expressions involved in the computations.

For example, the integral in all the exchange integrals which involves the integrand that multiplies either $G_o(1,x_1,\sigma_1,0,0)$ or $G_o(0.5-\beta,\gamma+x_1,r_1,q_j,m_j)$ vanishes identically if $\gamma=\eta=0$ and $h_k=q_k=0$. Similarly, both $G_k)_{direct}$ and $K_{jk})_{direct}$ vanish identically if $\gamma=\eta=0$ and $h_k=q_k=0$. In these cases, numerical values ranging from 10^{-9} to 10^{-12} were obtained. For corresponding non-zero similar type integrands, numerical values ranging from 10^{-1} to 10^{-2} were obtained. This indicates an accuracy of at least 8 significant digits

for this type of numerical integration.

By setting $\beta = 0$ and $m_k = 0$, the integral involving the infinite sum of a product of J_ℓ's may be analytically evaluated. It was found that the numerical value agreed with the analytical value to at least 8 significant digits. A further test relied on the symmetry property of the integrand containing an infinite sum of either a product of G_ℓ,s or a product of J_ℓ's. Here it was noticed that the appropriate integral values agreed with each other to at least 5 significant figures.

At first, some of the calculations were attempted using the DEC-PDP10 at the University of Western Ontario. However, it was found that the 36-bit word length of the PDP10 did not provide enough accuracy. All of the final results were done using Control Data Corporation Cyber 73/14 computer system (originally of the CDC6400 series) at the University of Western Ontario. This computer has a 60-bit word length, giving 14 significant figures for single precision.

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